CHAPTER 3
TOTAL SYSTEM PERFORMANCE

ANALYSIS TECHNICAL BASIS DOCUMENT
THERMAL HYDROLOGY

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Civilian Radioactive Waste Management System
Management & Operating Contractor

Chapter 3
Total System Performance Assessment-Viability Assessment (TSPA-VA) Analyses Technical Basis Document

Thermal Hydrology

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ACRONYMS

AML	areal mass loading
APD	areal power density
BWR	boiling water reactor
CAM	corrosion allowance material
CCDF	complementary cumulative density function
CRM	corrosion allowance material
CSNF	commercial spent nuclear fuel
DDT	discrete-heat-source, drift-scale, thermal-conduction (model)
DDTH	discrete-heat source, drift-scale, TH (model)
DFM	discrete fracture model
DKM	dual permeability model
DMTH	discrete-heat-source, mountain-scale, thermal hydrologic (model)
DOE	U.S. Department of Energy
DST	drift-scale test
EBS	engineered-barrier system
ECM	equivalent-continuum model
EIS	Environmental Impact Statement
ESF	Exploratory Studies Facility
G-ECM	generalized-equivalent continuum model
HLW	high-level waste
IRSR	Issue Resolution Status Report
KTI	key technical issue
LBNL	Lawrence Berkeley National Laboratory

LBT	large-block test
LDTH	line-averaged-heat-source, drift-scale thermal hydrologic (model)
LDTH-S	line-averaged-heat-source, drift-scale, TH, seepage (model)
LLNL	Lawrence Livermore National Laboratory
LML	lineal mass loading
LMTH	line-averaged heat source, mountain-scale, thermal-conduction (model)
LTA	long-term-average
MTU	metric tons of uranium
NFE	near-field environment
NRC	Nuclear Regulatory Commission
PA	performance assessment
PWR	pressurized water reactor
RIP	Repository Integration Program (computer program)
SDT	smeared-heat source, drift-scale, thermal-conduction (model)
SDTH	smeared-heat source, drift-scale, TH (model)
SHT	single-heater test
SMT	smeared-heat source, mountain-scale, thermal-conduction (model)
SMTH	smeared-heat source, mountain-scale, thermal-hydrologic (model)
SNF	spent nuclear fuel
SZ	saturated zone
TBV	to be verified
TEF	thermal effects on flow
TH	thermal hydrology or thermal-hydrologic
THC	thermal-hydrologic-chemical

THM	thermal-hydrological-mechanical
TSPA	Total Systems Performance Assessment
TSPA-VA	Total Systems Performance Assessment—Viability Assessment
UZ	unsaturated zone
YMP	Yucca Mountain Project

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3. THERMAL HYDROLOGY

3.1 INTRODUCTION

3.1.1 Overview

3.1.1.1 The Importance of Thermal Hydrology to Waste Emplacement in a Geologic Repository

The Yucca Mountain Project (YMP) is planning to emplace, in a geologic repository, radioactive wastes that will emit a significant amount of radioactive decay heat. This heat will influence hydrologic, mechanical, and chemical conditions in both the near-field and the far-field. The degree of heating will be a function of the repository areal mass loading. For the 85 metric tons of uranium per acre (MTU/acre) areal mass load currently considered by the project, the heat transfer processes will influence the repository and surrounding environment for many thousands of years after the emplacement of heat-generating wastes. The primary emphasis of the studies associated with thermal perturbations for the Total Systems Performance Assessment-Viability Assessment (TSPA-VA) has been on the thermal-hydrology (TH). Thermal-hydrology is defined as a physical change to the fluid components and host rock of the system driven by a heat addition. This includes quantification of the development of dryout and condensate zones resulting from heat addition, including a description of condensate shedding through the fracture system of the mountain around the emplacement drifts during the initial and full heating periods (see Figure 3-1 and Figure 3-2). This is achieved with the application of conceptual descriptions of physical processes that do not restrict fracture flow. Thermal-hydrologic analyses for the viability assessment also include quantification of large-scale gas-phase convection through the fracture system surrounding the emplacement drifts.

As noted above, *thermal-hydrologic* processes are the focus of the base-case calculations for the TSPA-VA TH component. Preliminary modeling sensitivity studies have been performed for TH processes weakly coupled to thermal-mechanical processes and strongly coupled to thermal-chemical processes. Based on these limited studies, near-field predictions made by TH-only models do not differ greatly from currently available results from simplified models including chemical dissolution-precipitation reaction equations (see Section 3.6.8). Additionally, predictions of the liquid-phase flow fields below the repository horizon made by TH-only models do not differ greatly from the results of a TH analysis, including weakly coupled, mechanical interaction between fracture aperture and fracture flow properties (see Section 3.6.8). However, uncertainties still exist in the simplified coupled-calculations (for example, how a precipitation cap near the emplacement drift influences the flow of water through fractures or the interaction between fractures and matrix rock) performed to date. Therefore, additional sensitivity studies will be necessary for the license application Total Systems Performance Assessment (TSPA). In order to aid in the reduction of uncertainties associated with coupled processes driven by thermal loading, the project established an expert elicitation to consider rock response to changes in chemistry and mechanical stresses.

The Near-Field-Environment Expert Elicitation (CRWMS M&O 1998) was established because of the uncertainties associated with thermal-hydrologic-mechanical (THM) and thermal-

hydrologic-chemical (THC) processes. The panel was specifically tasked with investigating how these processes occur, both temporally and spatially, and over what range of values the hydrologic properties (for example, fracture permeability) may be influenced.

The elicitation panel examined the most recent project process models as well as experimental data on coupled processes from the single-heater test. They considered THM and THC processes, potential changes to interactions between fractures and matrix rock, and effects of rock falls, with an emphasis on how rock falls influence TH conditions in the rubble within a drift. The panel found that fracture-permeability changes may occur in both the vertical and horizontal directions and in condensate and boiling zones. According to the panel experts, the change in fracture permeability in the vertical direction, depending on spatial location, can range from a decrease by a factor of 100 or an increase by a factor of 1,000. Fracture permeability in the horizontal direction may increase by as much as ~10 times. Based on the results of the elicitation, the potential for thermally driven alteration of fracture properties (for example, permeability) falls within the range of natural variability of the natural heterogeneity of the system. However, the thermally driven component of fracture alteration may tend to push this range toward the smaller values of fracture permeabilities. The panel concluded that, with the possible exception of horizontal changes in permeability resulting from shear stress, most mechanical effects will tend to be reversible upon cooling. They also concluded that chemical effects will be more permanent. The panel indicated that the fracture-matrix interaction parameter (X_{fm}, see Section 2.4.3.3.1 in Chapter 2 of the TSPA-VA Technical Basis Document for a general description of the parameter) used in the dual-permeability models may also be affected because of chemical precipitation or dissolution processes. This effect may be permanent; however, the range of change of this parameter is unclear because of uncertainties associated with heating processes and subsequent chemical interaction of water and fracture coating in the fractures. The mentioned uncertainty driven by thermal-chemical coupling is in addition to the uncertainty already associated with this parameter under ambient conditions alone.

The expert-elicitation results and the preliminary modeling studies of THM and THC processes are the bases for not including coupled-process effects in the TH analyses for the TSPA-VA base case. The models used to calculate fluid flow driven by heat are uncoupled from mechanical and chemical processes. This assumption requires further study.

Gaining an improved understanding of the TH processes has been considered to be a critical first step in modeling the thermal effects of the potential repository. The development of an appropriate conceptual model for TH flow has benefited a great deal from data and modeling activities associated with small- and intermediate-scale tests that have been conducted at Yucca Mountain (for example, single heater test and large block test). Future thermal test work may provide more information on the relative importance of thermal-mechanical and thermal-chemical (with respect to thermal-hydrologic) processes.

The potential repository horizon, located in the unsaturated zone (UZ) at Yucca Mountain, contains in situ pore liquid water and gas that will be affected by emplacement of heat-generating radioactive wastes. In general, the influence of radioactive decay heat includes: (1) vaporization of in situ liquid water, (2) thermally driven water vapor movement (primarily) away from the heat source, (3) condensation of water vapor in cooler regions, and (4) condensate

flow, driven by gravity and capillary forces. Thermal hydrology drives processes at two different physical scales. The thermodynamic environment in the emplacement drift is strongly dependent on the decay-heat characteristics from each of the individual waste packages in an emplacement drift. Quantification of the thermodynamic environment within the drift provides a description of the conditions in the drift (e.g., hot, dry, humid) and surrounding the waste packages. This description includes temperature, relative humidity, air mass fraction, and fluid flow time-histories near the waste packages and into the drift. The resulting thermodynamic conditions within the emplacement drift contribute to the performance of the repository by influencing the performance of the emplaced waste packages. After the emplacement of heat-generating wastes, thermal energy will flow through the mountain from the repository by conduction and convection heat-transfer processes. Vaporization of water driven by repository heating is expected to cause the formation of temporally and spatially varying dryout and condensate zones, with subsequent transport of water vapor, liquid water, and latent heat. Water may also flow (drain) preferentially downward through a connected fracture network between emplacement drifts.

The heat transfer processes described above will result in elevated temperatures of the host rock surrounding the repository. Subsequently, the properties of the rocks in the UZ will change, resulting in changes in the ambient hydrology and fluid flow conditions of the mountain. Large-scale heat flow will alter flow fields below the repository to the saturated zone (SZ). As a result of elevated temperatures, chemistry, or other mechanical processes, alterations in the porosity, permeability, and capillary pressure relationships can occur in the layers located below the repository. Changes to the hydrologic properties of the system include, among other things, a reduced liquid-phase relative permeability in the dryout zone (Francis et al. 1997b), Figure 7. Changes analogous to the latter are expected to have larger impacts on the thermally driven flow fields. Neglecting any potential changes to the flow properties as a result of processes other than hydrologic-only, the thermal perturbation itself influences the water and gas flow field for only a few thousand years (see Section 3.5.5.1 for mountain-scale flow fields resulting from heat) after the emplacement of waste. In the drift, neglecting changes other than hydrologic, thermodynamic conditions (temperature and relative humidity) in and around the waste packages return to nearly ambient conditions after about 100,000 years (see Section 3.5.5.2)..

The models used in the TSPA-VA to represent TH processes include an explicit determination of heat-driven processes occurring in both the near field (processes occurring at the scale of a waste package and emplacement drift) and in the far field (processes occurring at the scale of the entire repository and mountain). Thus, TH models provide the tools to make judgments as to the nature and the extent of the thermal perturbation of the water and gas phase flow fields in the entire UZ as well as in the thermodynamic environment within the emplacement drifts. The importance of this differentiation is discussed further in the next section.

3.1.1.2 The Importance of Scale to Thermal-Hydrology

The thermodynamic environment within the emplacement drift is related to the drift and waste package geometry, waste package spacing and sequencing, drift-to-drift spacing, and individual waste package heat outputs. The TSPA-VA TH model that includes this level of detail is referred to as a drift-scale model, since it includes features at the scale of the waste packages and surrounding emplacement drift. Individual waste package types in the drift-scale model include

different commercial spent nuclear fuel (CSNF) waste packages, codisposal including the defense high-level waste (HLW) glass, and separate disposal of Department of Energy (DOE) spent nuclear fuel (SNF) (direct disposal) containing varying numbers of DOE SNF. The TH models at the scale of the drift account for the potential package-to-package variability and how individual waste packages interact with each other, with the surrounding drift wall, and with the concrete liner and invert. The initial heat output of waste packages in the drift-scale models ranges from the coldest (0.8 kW) separate disposal waste package to the hottest (18 kW) design basis CSNF waste package.

As described above, the emplacement of heat-generating wastes in the repository alters large-scale fluid and heat processes associated with the scale of the mountain. TSPA-VA TH models that include heat release from the entire repository block are referred to as mountain-scale models. Heat-driven features at this scale potentially include the development of large-scale gas-phase buoyant convection cells and thermally altered liquid-phase flow fields both above and below the potential repository. Regions of dryout with associated condensate drainage may occur on a repository scale. The determination of how the liquid-phase flow field is thermally altered during and after the thermal perturbation is necessary for a complete description of radionuclide transport from the repository to the SZ.

Models at the scale of the mountain treat the total thermal load as being spatially uniform throughout the repository. The decay heat output of the potential repository is based on an average of the total number of assemblies of the two major types (boiling water reactor [BWR] and pressurized water reactor [PWR]) of CSNF, a blended HLW glass-waste heat output, and the major heat component of the DOE SNF. The total thermal output of the potential geologic repository at Yucca Mountain is obtained by assuming emplacement of 63,000 MTU of commercial spent nuclear fuel, 4,667 MTU of HLW, and 2,333 MTU of the DOE SNF waste. For the base-case areal mass loading of 85 MTU of CSNF/acre, the heated repository area is approximately 741 acres or 3 km^2. This corresponds to the dimensions of the western block of the potential repository (see Figure 3-3).

3.1.1.3 Inputs to Other TSPA Models from Thermal-Hydrology

Thermal hydrology base case and sensitivity results serve as inputs to near-field and far-field models used in TSPA-VA. The near-field TSPA models that receive input from TH are (refer to Table 3-1 and Figure 3-4):

- *Near-field geochemical environment*—temperature, air mass fraction, gas-phase flow rates (both vertical and horizontal) at the drift.
- *Waste package degradation*—surface temperature of the waste package, relative humidity of the waste package surface, water seepage into emplacement drifts and onto waste packages.
- *Waste form degradation*—temperature of the waste package, water seepage into emplacement drifts and into waste packages.
- *EBS transport*—liquid saturation of the concrete invert.

The form of this product is a time-history response curve after the emplacement of heat-generating waste.

Thermal-hydrologic model results also provide an assessment of the liquid-phase flow field below the repository during the thermal perturbation. This is required in order to assess the impact of the thermal perturbation on the UZ flow fields used in the radionuclide transport calculations in the UZ.

3.1.1.4 Inputs to Thermal-Hydrology From Other TSPA Models

Inputs to TH modeling came from the UZ-flow and disruptive-events components of TSPA-VA. The hydrologic parameters were defined within the UZ-flow task. Climate information was defined within the UZ-flow (infiltration rate over time) and (water-table height over time) task. Climate change information provided infiltration rates at the surface boundary for both drift-scale and mountain-scale TH models used in the TSPA-VA analyses. Rockfall scenarios were defined within the disruptive-events task. Rockfall is caused by thermal-mechanical and seismic stresses and will effectively add a rubble backfill in the emplacement drifts. This will change both the thermal and hydraulic properties of the drifts sometime between a few hundred to a few thousand years after waste emplacement. The thermal-hydrologic response obtained from a drift-scale rockfall model is required for a reference repository design not including an engineered backfill at closure.

A rockfall event after the emplacement of heat-generating wastes is considered as a sensitivity study for a repository design using non-backfilled emplacement drifts. The mechanics of the process are not specifically considered, only that rockfall will occur and with a varying range of parameters that may describe the physical conditions in the drift after wall collapse. The results of this analysis are given in Section 3.6.6. This analysis is carried out with respect to TH only and is meant to estimate the thermal and hydrologic environment in a rubblized zone surrounding the waste packages after rockfall occurs at a specified time. It does not consider influences on the waste package other than contact of a different surrounding environment after the drift wall collapses. Mechanical damage (if any) to the waste package as a result of rockfall is not considered in the analysis. Parameter inputs for the TH rockfall analysis including fill porosity, effective fill permeability, and fill height, are obtained from ranges of values developed from the Near-Field-Environment Expert Elicitation (CRWMS M&O 1998, pp. 3-7 of 23 and 3-8 of 23).

3.1.2 Previous TSPAs

For TSPA-1993, thermal calculations were performed using a conduction-only model (Wilson et al. 1994). Three-dimensional drift-scale and mountain-scale calculations were performed for two initial thermal loads (57 and 114 kW/acre). Effects on the hydrology (e.g., the extent of dryout) were inferred from the extent and location of the boiling isotherm. For the drift-scale calculations, periodic boundary conditions were applied to a single waste package (thus creating an effectively infinite repository) and drifts were assumed to be backfilled 75 years after waste emplacement, using gravel with an effective thermal conductivity of 0.2 W/m-K. Before backfill, radiant heat transfer in the empty drifts was approximated by an enhanced thermal conduction with an effective thermal conductivity of 20 W/m-K. The drift-scale calculations were used to model early-time behavior only. At late times (different for center or edge waste

packages), an analytical solution was used instead of the periodic-cell model. This allows for reduced temperatures in response to the finiteness of the repository (e.g., edge effects). In the analytical-solution modeling, irregular waste streams and sequential emplacement of waste were also considered. Waste package temperature, dryout volume, and fraction of dry-waste packages, as functions of time, were derived from the thermal modeling and used for modeling seepage into drifts and waste-package and waste-form degradation.

For TSPA-1995 (CRWMS M&O 1995), two-dimensional drift-scale TH calculations were performed for two different areal mass loads (25 and 83 MTU/acre), using the equivalent-continuum model (ECM) assumption for heat and fluid flow. Infiltration rates of 0.05 and 0.3 mm/year were modeled for a laterally homogeneous layered system. The model domain was a column within the UZ from the ground surface to the top of the water table and from the drift center line to the center line between drifts. This results in a periodic model domain representative of the center of the repository. Cases with and without backfill were modeled. For cases with backfill, drifts were assumed to be backfilled using gravel with a thermal conductivity of 0.6-W/m-K, 100 years after waste emplacement. For nonbackfilled drifts, radiant heat-transfer effects were modeled explicitly. Because of the periodic boundary conditions, the modeled (drift-scale) repository was effectively infinite in extent. A scaling concept was introduced in order to simulate a waste package located near the edge of the repository. This was described as a solution matching technique using two-dimensional models and the results of a "tuned with respect to heat output" one-dimensional model. That is, the heat output in a one-dimensional mountain-scale model is reduced so that its solutions "look" more like the solutions that occur at the edge of the two-dimensional model. The "scaling" factor used to reduce the thermal output of the one-dimensional model can then be applied to the drift-scale model. The edge response is then identical to that of the center, only at a lower thermal loading. However, this scaling concept was not used in the TSPA-95 calculations. The time-histories for the waste package temperatures and relative humidities for only the center model were used for modeling waste-package and waste-form degradation.

3.1.3 Current Treatment of Thermal-Hydrology in Support of TSPA-VA

3.1.3.1 Improvements in TSPA-VA Thermal-Hydrologic Models

Thermal hydrology models describe the physical processes occurring in the natural geologic system as well as in the engineered barrier system (EBS). The location of the thermal perturbation is often referred to as the "altered zone" as a result of repository decay heating. The performance of the potential repository must include an appropriate description and a reasonable assessment of the TH conditions in the near-field, far-field, EBS, and at the waste package surface. Phenomena such as dryout and relative humidity reduction, ambient and nonisothermal seepage, water vapor movement in the gas phase, and alteration of rock properties resulting from coupled processes will all influence, to varying degrees, the TH predictions made by the process-level models.

Improvements in the TH modeling for the VA included the areas of conceptual flow models, large-scale heating responses, and waste package variability expected at the repository:

- Large-scale effects as a result of repository heating

- Edge cooling responses
- Gas-phase flow vertically driven by buoyant forces
- Development of dryout and condensate zones

- Waste package variability of
  - Commercial waste forms
  - Additional waste forms

- Alternative conceptual flow models that allow
  - Increased rate of fracture flow near drifts
  - Higher infiltration rates at the ground surface, including climate changes.

The thermal models used in support of TSPAs have increased in complexity since they were first included in TSPA-93. With the development and recent testing of new conceptual models governing heat and mass flows, the institution of the Yucca Mountain Project thermal-testing programs (both laboratory and in situ field-testing), and the growth of the project knowledge base through workshops and expert elicitations, TH modeling of a potential geologic repository at Yucca Mountain has become increasingly more refined and less dependent on broad-based assumptions. A description of the newer features included in the VA TH models is highlighted below, with the details of the analyses given in subsequent sections in the TH chapter.

The TH models used in support of the TSPA-VA (for example, see Table 3-2) include multi-dimensional (one-, two-, and three-dimensional) mountain-scale models that represent most large-scale features of the potential repository site. The two-and three-dimensional models used in the TSPA-VA included the actual topography of the mountain surface, variations in stratigraphy as specified in the UZ-flow site-scale model (see Section 2.4.3.8 in Chapter 2 of the TSPA-VA Technical Basis Document), repository-scale thermal loading including edge cooling effects, and the natural development of large-scale buoyant gas-phase convection as a result of fluid density variations in a gravitational field. Table 3-2 indicates the salient features of previous TSPAs as well as those in the current TSPA.

Although previous TSPAs made an attempt to account for the large-scale edge cooling effects, it did not account for the large-scale gas-phase effects (e.g., gas-phase flow and how the effects relate to the development of the air mass fraction near the repository drifts) either by application of conduction-only models (TSPA-93) or by application of a gas-flow limited, two-dimensional, periodic, drift-scale model (TSPA-95). TSPA-VA TH models capture large-scale effects related to edge cooling of a finite repository and the development of large-scale gas-phase flow patterns that move water vapor and heat by a nondiffusive mechanism. Vertical fracture property descriptions that govern the thermally driven flow fields are obtained from recent field data associated with pneumatic testing data (see Section 2.4.3.1 in Chapter 2 of the TSPA-VA Technical Basis Document).

Perched water zones exist below the repository horizon in some parts of Yucca Mountain. The perched water zone can serve as a mechanism for lateral flow towards the east below the repository. TSPA-VA TH and conduction-only mountain-scale models did not include the naturally occurring perched water zones below the repository since the thermal perturbation to

the mountain flow field is short lived (refer to Section 3.5.5). Also, any perching of (heat driven) water that may occur in response to thermally driven chemical changes to the system are not included since thermal-hydrologic-chemical processes are not directly included in the base case TH analysis. (This is a topic for future study during the abstraction and testing analyses for the license application.) Finally, the one-dimensional model column inversions used to develop the hydrologic property sets did not include the influence of natural perching below the repository. Since the drift-scale models used in TH analyses are column-like as well, they did not incorporate naturally occurring perching.

Model advancements for the VA are not limited to the large-scale TH models. Improvements have been made to the waste package-scale TH models as well.

In TSPA-93, since conduction-only models were used, moisture impacts as a result of repository heating were inferred from temperature results alone. In TSPA-95, the two-dimensional TH drift-scale model was limited by reduced dimensionality along the drift and could only assess the relative humidity and temperature for an average fuel and waste package type.

TSPA-VA drift-scale TH models (one-, two-, and three-dimensional) were developed in order to describe TH responses (temperature, liquid saturation in invert, relative humidity at the waste package, etc.) at the scale of the drift wall and waste packages. This included quantification of the variability of heat output from package-to-package for different waste package types emplaced in the repository drifts. Previous TSPA TH models could not include waste package variability and the processes driven by this variability as a result of single waste package models (TSPA-93) or application of two-dimensional drift-scale models that axially smeared heat in the dimension along the drift (TSPA-95). The TSPA-VA TH analyses at the scale of the drift provide a better representation of the different waste packages emplaced in the repository drifts as it approximately accounts for the actual percentages of the total allotment of each waste package type and associated heat outputs. The TSPA-VA models specifically included different commercial fuel types (both BWR and PWR) as well as HLW and DOE SNF wastes. The TSPA-VA improvements associated with model scale have been briefly described. Associated details embedded within the TH models, such as waste package sequencing and spacing, heat loading of each of the individual waste package types or for the entire repository, etc., will be given in upcoming sections (refer to Section 3.5.3). Improvements related to the conceptual models of fluid and heat flow applied to the TH models used in support of TSPA-VA will also be introduced in this section.

Past TSPA TH analyses assumed either no fluid components (TSPA-93) with heat transport by conduction-only, or an ECM flow model (TSPA-95) governing heat and fluid transport in a fractured-porous medium. TSPA-93 used three-dimensional drift- and mountain-scale conduction-only models. Therefore, convection of heat (sensible and latent) was not included and hydrologic response was inferred from the resulting conduction-based temperature distributions alone. TSPA-95 used an ECM flow model governing both heat and mass transfer in the two-dimensional drift-scale TH model. The ECM assumption is typically applied because of the computational efficiency required when solving both conservation of energy and conservation of mass. TH models are computationally rigorous because of the required solution of both mass and energy equations. Numerical difficulties arise, in particular, because there is a change of phase of the water constituent during heating. The Nuclear Regulatory Commission

(NRC) has indicated that obtaining fracture water flow while still using the computationally efficient ECM would be necessary in future TSPAs (Baca and Brient 1996, pp.4-9). The issue of conceptual fracture flow model is addressed in TSPA-VA by application of the equivalent continuum model (G-ECM) abstraction testing. Mountain-scale models are used primarily to obtain gas-phase information such as air mass fraction and gas-phase flow rates at the repository horizon. This need is less dependent on liquid fracture flow processes since gas-phase flow occurs in the fractures where fracture liquid saturations are generally quite low. The ideal approach is to apply a dual permeability model for fractures and matrix rock. This approach is applied to the TH multiscale modeling and abstraction method used to obtain the thermodynamic response of the repository at the scale of the drift and waste package. The TH multiscale modeling and abstraction method is used to obtain base case and sensitivity study results. Each of the conceptual flow models applied to the TH process-level models (mountain and drift-scale) resulted in increased fracture flows as described throughout this document (refer to Section 3.4.2). A simplified discussion of each is given in the following paragraphs.

The ECM assumption implies capillary pressure and thermal equilibrium between fractures and matrix, with the resulting composite material made up of fracture pore volume weighted fracture and matrix properties. This is equivalent to having an "infinite" conductance between fracture and matrix rock with the majority of liquid flow occurring very slowly in the matrix. This flow model assumption has been found to limit water flow through fractures until the matrix rock is almost completely saturated. It has been shown in previous studies (Ho et al. 1996b, pp. 6-5 and 6-7) that condensate drainage occurs in fractures during the formation of the dryout zone. Drainage through the fractures can proceed even if the matrix block is not fully saturated. In order to reduce the potential error related to the initiation of fracture flow inherent in the standard ECM formulation, both G-ECMs and dual permeability models (DKM) have been used as alternative conceptual flow models during the repository heating and cooling process.

Like the ECM, the G-ECM conceptual model adheres to the same assumptions of capillary pressure and thermal equilibrium between fracture and matrix. In the G-ECM, the matrix satiation saturation is reduced (to something less than fully saturated), which will permit "fracture" flow to occur. To achieve this, the capillary pressure in the matrix block approaches zero at the lower matrix satiation saturation value. The process of allowing fracture flow before the matrix is fully saturated is equivalent to saying that the matrix rock contains an irreducible gas-phase component within its pore space.

Reducing the matrix satiation saturation also allows for a TH analysis with much higher infiltration rate boundary conditions without saturating the entire model domain. Although improved, this conceptual flow model is still limited within the dryout zone because of the forced equilibrium between the fractures and the matrix rock. The DKM conceptual flow model allows for fracture and matrix rock domains to be in disequilibrium. It allows for a finite mass transfer rate between fracture and matrix. Liquid water transport may occur in an entirely separate fracture and/or matrix domain. It is also possible that flow may occur between fracture and matrix rock. The issues related to coupling and quantitatively describing wetted flow areas between fracture and matrix have been explored in Section 2.4.3.3 in Chapter 2 of the TSPA-VA Technical Basis Document. For the current TSPA TH analyses, the G-ECM conceptual flow model was applied in the two-dimensional mountain-scale and three-dimensional drift-scale TH model (this drift-scale model is the testing model). The DKM was applied to the two-

dimensional line-averaged-heat source, drift-scale, TH model used in the TH multiscale modeling and abstraction method. The standard ECM is used only in Section 3.4.5 in the comparison to single heater test measured data. All other TH analyses use the DKM or G-ECM conceptual flow models.

3.1.3.2 An Overview of the Thermal-Hydrology Multiscale Modeling and Abstraction Method for TSPA-VA

Drift-scale modeling must include more processes than just those occurring at the drift scale. The drift-scale processes must be coupled to mountain-scale processes in order to properly show that waste packages near the edge of the repository cool off faster than waste packages near the repository center. A multiscale modeling and abstraction method was developed to couple drift-scale processes to mountain-scale processes. This method uses a series of four mountain-scale and drift-scale submodels to abstract the thermodynamic environment within the repository drifts at a variety of different repository locations. The submodels are illustrated in Figure 3-5.

(1) The *line-averaged-heat-source, drift-scale, thermal-hydrologic (LDTH) submodel* (see Section 3.5.1.4.3 for more details) is a two-dimensional drift-scale model that computes average temperature and relative humidity at the drift wall. This submodel includes the hydrologic processes (for example, surface infiltration rates and different climate states, hydrologic properties, and dual-permeability-model concept of heat and fluid flow) and parameters used to describe a location, given specific coordinates within the repository. It is also used to compute the average liquid saturation in the drift invert. The flow is modeled as dual permeability, consistent with the mountain-scale, unsaturated-zone flow model (refer to Section 2.5.1 in Chapter 2 of the TSPA-VA Technical Basis Document). Radiant heat transfer within open drifts is modeled explicitly. This submodel addresses the key issues listed in Section 3.3 for appropriate modeling of fracture and matrix rock interactions for fluid and heat flow. It also addresses methods for upscaling (accounting for difference between small-scale experiments or observations applied to larger-scale features) of fracture properties and TH processes by including the hydrologic properties developed by inversion models described in Section 2.4.3.1 in Chapter 2 of the TSPA-VA Technical Basis Document. The coupling to the mountain-scale, unsaturated-zone flow model ensures that hydrologic conditions at Yucca Mountain are properly accounted for, including spatial variability of infiltration and changes of infiltration with climate.

Next in the abstraction process are the (2) *smeared-heat-source, mountain-scale, thermal-conduction (SMT) submodel* (see Section 3.5.1.4.1 for more details) and the (3) *smeared-heat-source, drift-scale, (SDT) thermal-conduction submodel* (see Section 3.5.1.4.2 for more details). Both are models solely for conduction. These submodels are used to establish temperature relationships and to account for the influence of repository edges, topography, and mountain-scale variability in hydrogeologic layering. The smeared-heat-source, mountain-scale submodel is a three-dimensional model that includes the appropriate stratigraphy, topography, and repository location and extent. The smeared-heat-source, drift-scale submodel is a one-dimensional model. These two submodels address key issues related to the differences between repository "center" and "edge" locations by coupling the drift-scale submodels with the mountain-scale submodel. The coupling is done as follows. The average temperatures of repository host rock obtained from the smeared-heat-source, mountain-scale submodel are corrected for hydrology using a relationship derived from the line-averaged-heat-source, drift-

scale submodel and the smeared-heat-source, drift-scale submodel. The resulting "modified" temperatures inherently include edge effects because they originated from a full mountain-scale model. Additionally, the temperature prediction includes the effects of the system's fluid components through a temperature relationship developed between the two drift-scale submodels. This procedure results in an "abstracted" drift-wall temperature that approximates the effects of the most important TH processes. An analogous procedure is followed to determine an abstracted relative humidity at the drift wall.

The abstracted drift-wall quantities are further modified at the drift wall and at the waste-package surface using waste-package-specific deviations computed by the (4) *discrete-heat-source, drift-scale, thermal (DDT) submodel* (see Section 3.5.1.4.4 for more details) to obtain temperatures and relative humidities for different waste-package types along the drift. The discrete-heat-source, drift-scale submodel is a three-dimensional model of a drift segment containing seven representative waste packages of varying heat outputs. This submodel includes only conductive heat transfer, plus radiant heat transfer within open drifts. It accounts for variability in temperature and relative humidity among packages along the drifts, which is one of the key issues listed in Section 3.3.

The above process steps are performed for a number of repository locations. For a given drift-scale-model calculation, there is only one computer run of the mountain-scale submodel, but the line-averaged-heat-source, drift-scale TH submodel is run for a matrix of 35 different locations (see Figure 3-3) within the repository block. This total (35 select locations) provides north-south and east-west coverage over the entire repository block. It includes model locations with different infiltration rates, stratigraphy, and repository host rock. The abstracted temperature and relative humidity are calculated for a matrix of 425 repository locations (from the SMT model), giving reasonable spatial resolution for incorporating mountain-scale topographic and stratigraphic effects. The 35 drift-scale locations are a subset of the 425 repository locations. That is, the repository heated footprint encompasses 425 grid blocks. The drift-scale model locations (35 total) fall within these locations. The results of drift-scale models are interpolated from location to location so that all 425 locations may approximate repository heating effects including hydrology. However, this procedure provides too much information to be used by the near-field TSPA-VA components. Because resource demands increase linearly as the number of waste-package groups modeled within RIP (Repository Integration Program, the top-level TSPA computer program) increases, we determined that six repository subregions are sufficient for modeling the near field with RIP, as shown in Figure 3-6. From a TH standpoint, six regions are expected to account for variability around the repository since the selected zones included regions of high-to-low infiltration rates, different repository locations (for example, center and edge), and different repository host units. The division is based primarily on infiltration rate at the ground surface (that is, the division minimizes infiltration variability within subregions as much as possible, although there is still considerable variability). The subregions also represent a range of geometric relations (for example, proximity to the repository edges), with Region CC being the subregion most like the repository center and Region SW being most like the edge. Lastly, the subregions represent the variation of hydrogeologic properties around the repository. The reference repository cuts across three hydrogeologic units, the Topopah Spring Middle Nonlithophysal, Lower Lithophysal, and Lower Nonlithophysal units. Region SW is mostly in the Lower Nonlithophysal; Regions NW, NE, CC, and SC are mostly in the Lower Lithophysal; and Region SE is mostly in the Middle Nonlithophysal. Each of the 35 drift-scale model

locations (described above and used in the TH multiscale modeling and abstraction method) falls within the six repository subregions. Each subregion may contain approximately five to six drift-scale model locations.

The results from modeling approaches containing drift-scale analyses are time-histories of waste-package temperature and relative humidity, drift-wall temperature and liquid saturation, and invert-floor temperature and liquid saturation.

3.1.3.3 A Discussion of the Testing Approach for the Thermal-Hydrology Abstraction Methodology

This modeling process includes multiple scales (mountain and drift), multiple dimensions (one, two, and three dimensions), and varying assumptions regarding the coupling of heat transfer to fluid flow (conduction-only and full thermal-hydrologic). To provide greater confidence that the TH multiscale modeling and abstraction method described above adequately represents the TH behavior of the Yucca Mountain repository, an independent model was developed. The model incorporates three-dimensional, fully coupled heat transfer and fluid flow but uses a less mechanistic conceptual flow model (G-ECM rather than DKM) and a less sophisticated coupling between drift scale and mountain scale. It uses abstracted information from mountain-scale, TH models to approximate edge effects. The computational requirements of the verification model do not allow the many abstraction simulations that are required for a total-system calculation. However, this type of model provides a check on the previously described abstraction processes. Good agreement was found when the independent approaches were compared at repository center and edge locations. This analysis addresses the key issue of the importance of tradeoffs between model dimensionalities. We conclude, based on this comparison, that the combination of one-or two-dimensional models with reduced complexity in heat-transfer models suffices for determining near-field responses associated with waste-package heating. This simplicity provides flexibility in producing the many simulations required of a total-system performance assessment.

3.1.3.4 Mountain-Scale Thermal Hydrology

Determining the development of mountain-scale gas-phase flows in response to thermal loading requires a different modeling approach than the one described above used to obtain drift-scale performance characteristics. Mountain-scale TH models are used to calculate quantities such as air mass fraction and gas-phase fluxes associated with larger scales. The TH multiscale modeling and abstraction method described previously is unable to account for gas-phase advection that results from large-scale temperature and pressure gradients because only conduction is included in its mountain-scale submodel. At the mountain scale, gas-flow patterns that may result from repository heating can be achieved only with a fully coupled TH model. The key issue addressed by this model is the importance of using the dual-permeability model at the mountain scale (Section 3.3), in particular for modeling the movement of gas and liquid through fractures. A G-ECM flow model is used to determine gas-phase data for the mountain. Using this model reduces the computational requirements of the larger-scale TH simulations while still allowing for sufficient mobility of liquid water in fractures. The mountain-scale model is described below.

A mountain-scale model based on east-west cross sections is used for each of the property sets and associated infiltration rates considered in the TSPA-VA analyses (see Figure 3-3 for its location). The mountain-scale model includes large-scale features such as the mountain's topography and spatial variability of the infiltration rate at the ground surface. It also includes repository-edge effects and the ability to develop large-scale fluid-flow processes such as buoyant convection, in which fluid moves in response to a density gradient. The cross sections used to calculate gas flow were taken directly from the mountain-scale, UZ flow model (see Section 2.4.3.8 in Chapter 2 of the TSPA-VA Technical Basis Document). The model includes the stratigraphy and hydrologic properties established for the UZ flow model. The mountain-scale model includes the heat output of the entire repository waste stream (scaled for a two-dimensional application) simultaneously emplaced at the time of repository closure.

3.1.3.5 Form of the Thermal Hydrology Product

Figure 3-7 indicates the location of TH modeling data passed to other TSPA models. Figure 3-8 indicates which model formulation produces the data. The form of abstraction of UZ TH into TSPA-VA is a series of time-history tables (for example, temperature versus time) of far-field gas-phase flow rates and air mass fraction data as well as thermodynamic state variables within the emplacement drifts at six different repository subregions. Refer to Table 3-1 for model details.

Two-dimensional, mountain-scale, TH calculations provided the time-histories for gas-phase flow rates ($\dot{m}_{gas}$) and air mass fractions (X_{air}) at repository center and edge locations. Air mass fraction as well as vertical and horizontal gas-phase flow rates were obtained at the repository horizon from the models including large-scale features of the site from the UZ-flow site-scale model. All mountain-scale TH models were completed with the TOUGH2 flow code (Pruess 1991). TOUGH2 is capable of running TH simulations in ECM, G-ECM, and DKM formulations. The version of TOUGH2 used in the mountain-scale TH calculations was v. 3.4.2. It has been qualified under the YMP quality assurance program (SNL QAIP 19-1).

The TH multiscale modeling and abstraction method provided temperature ($T_{waste\ package}$) and relative humidity ($RH_{waste\ package}$) at the surface of the waste package, the drift wall temperature, ($T_{drift\ wall}$), and liquid saturation in the invert (S_{invert}). These quantities were provided for six representative repository subregions and for different waste-package types. The results were binned for different relative humidity and temperature responses. The PA "testing for model confidence" models at repository center and edge were used to validate the TH multiscale modeling and abstraction method at two locations, center and edge. NUFT is capable of running TH simulations in ECM, G-ECM and DKM formulations. The NUFT computer program (Nitao 1996) was used for all drift-scale TH calculations. The versions of NUFT used in the TH multiscale modeling and abstraction method as well as in the PA testing models were not qualified. The version numbers for the NUFT code are listed at the end of this section in Table 3-4.

3.1.4 A Discussion of the Issue Resolution Status Report by the Nuclear Regulatory Commission

The Issue Resolution Status Report (IRSR) is used by the NRC staff to provide the DOE feedback on any of the subissues making up the key technical issues (KTIs). For TH (U.S. NRC 1997) the thermal-effects-on-flow (TEF) KTI is focused on thermally driven redistribution of moisture caused by repository decay heat and temperature and relative humidity of the waste-package environment. The NRC then divides the KTI into three important subissues:

- Is the DOE TH testing program, including performance confirmation testing, sufficient to assess the potential for thermal reflux to occur in the near field?
- Is the DOE TH modeling approach sufficient to predict the nature and bounds of TEF in the near field?
- Does the DOE TSPA adequately account for TEF?

Based on TEF, the NRC identified four key elements of the engineered and natural subsystems:

- Waste package corrosion
- Quantity and chemistry of water contacting waste forms
- Fracture versus matrix flow
- Spatial distribution of flow.

The NRC defines thermal reflux as the redistribution of moisture driven by heat that could result in channeling moisture toward a waste package. The report then discusses how thermal reflux provides the interaction within key elements and between key elements listed above. Each is important to long-term performance of the potential repository. The NRC describes the importance of thermal reflux on the integrity of a waste container, the transport of radionuclides from breached waste canisters, and the alteration of hydraulic or transport pathways through the EBS. The NRC indicates that the primary sources of reflux water are from ambient rock waters and incident percolation waters and estimates that as much as 8,000 m^3 of water are vaporized per waste package, for thermal-loading scenarios that result in dryout zones 100 m above and below the repository horizon. This value (8,000 m^3) is somewhat higher than the values computed from the base case TSPA-VA TH analyses because the extent of the dryout zone (both above and below the drift) is substantially lower than that indicated by the NRC. Depending on infiltration rate, the dryout zone extent predicted in the TSPA-VA analyses is not more than about 15 to 25 m below the repository and ~15 m above for a hydrologic property set that allows the formation of an extended superheated zone by altering the matrix diffusivity parameters of the host rock units (Hardin 1998, p. 3A-22). The difference may in part be a result of the higher overall infiltration rates currently being applied to the TSPA analyses. Higher infiltration rates (as well as other hydrologic property attributes) impede the growth of the dryout zone during the thermal periods.

The report discusses the DOE's previous considerations of thermal reflux in previous TSPAs (TSPA-93, and TSPA–95) and reviews Iterative Performance Assessment Phase 2 (U.S. NRC 1997) with respect to this issue, discussing ongoing sensitivity studies based on the process-level model MULTIFLO and the abstracted models REFLUX1 and REFLUX2 in the Total System Performance Assessments (TSPA) code. Both models are used to assess the effects heat and mass transfer mechanisms may have in terms of sensitivity to dose. Thermal-hydrologic and thermal environments within the drift are obtained from the process-level model, while rates of refluxing water are obtained from the abstracted models.

The NRC report then reviews the methods and acceptance criteria for the three subissues listed above as being important to TEF. The acceptance criteria for each of the subissues include programmatic elements, technical and confirmatory elements, and a review method. Subissue 1 is related to the sufficiency of the DOE thermal testing program to provide information used to verify conceptual models used by the DOE to evaluate thermally driven flow in the near field. Subissue 2 is related to the sufficiency of the DOE TH modeling approach (e.g., process-level models) to predict thermally driven flow in the near field. Subissue 3 is related to the DOE demonstration of the adequacy of its TSPA with respect to TEF.

Finally, a status is given of subissue resolution at the staff level. Previous comments have been resolved at the staff level. However, the NRC has indicated that the staff will review the bases underlying the parameter values used in the TH analyses as well as parameter values used to describe the drift environment in the event of an engineered backfill scenario. Regarding liquid flows into the emplacement drift, the staff will review the bases underlying the amount, timing, and duration of liquid water contacting the waste packages after waste emplacement. Other NRC audit reviews considered additional restrictive assumptions and areas of concern in the DOE TSPA-95 and the thermal testing programs. The details of each are given in Section 5 of the U.S. NRC (1997).

Each of the three KTI subissues identified by the NRC was either considered or incorporated into the process-level models developed for the TH component of the TSPA-VA. The first subissue related to the thermal testing program questions concerning the ability of the YMP thermal tests to determine the amount or impact of the thermal refluxing processes (i.e., water flow through fractures/and or matrix rock as a result of vapor movement and condensation above and below the heat source). This issue was investigated recently by the project during the course of conceptual flow model validation exercises and hydrologic property set comparisons against the measured results of the single heater test (see Section 3.4.5). The hydrologic property sets used in the total system performance assessment calculations were used in an ECM and a DKM formulation of the single-heater test (SHT) experiment. Assessments were made regarding the suitability of individual property sets (the same as those used to generate the flow fields for the UZ transport calculations) to predict heat flow processes in the dryout and evaporation zones adjacent to the heat source. Some property sets do better than others. Additionally, assessments were made regarding the most appropriate conceptual flow models governing the TH flow processes. Based on the measured results of the SHT, it was determined that the DKM more accurately represents the thermally driven flow processes that occurred at the SHT. In particular, DKM was better able to model the water that flowed into the fracture domain and out of the system during heating.

The second KTI questions the ability of the process-level model to predict the nature and bounds of TEF in the near-field. Based on the results of the single heater test, it was found that the DKM more accurately represents the heating and fluid flow behavior because heat was added to a fractured porous medium. This result has been incorporated by the project into process-level descriptions of TH. Subsequently, the process-level models used to predict the performance attributes of the engineered barrier systems used conceptual flow models (for example, DKM) found to be in good agreement with the measured temperature results of the SHT. (Some additional property set and conceptual flow model comparisons can be made to the drift-heater test when these data become available [from the first 1.5 years of heating], in time for the license application).

Finally, the third KTI is associated with the implementation of TEF in the TSPA. This is accounted for inherently in the abstracted models if the conceptual flow model applied in the process-level model allows for disequilibrium fracture flows developed during the transient thermal period. Relative humidity in the drift originates from models that allow for increased fracture flows to and around the emplacement drifts. Temperature predictions, both drift-wall and waste-package surface, have been computed from a process-level model that allows for more water in fractures. As this fracture water travels through a connected path towards the drift, temperature and relative humidity predictions account for wetter conditions near the heat sources.

3.1.5 An Outline of Chapter 3

Section 3.2 of this TSPA-VA Technical Basis Document provides a basic discussion of the process-level models used in TH for previous TSPA calculations and post-TSPA-95 TH analyses. This section also provides a highlight of the details of our (PA) understanding of the TH processes/issues as we proceeded into the abstraction/testing workshops. Each workshop was designated by the DOE as the basis for developing the processes and issues that would be associated with, and addressed by, the TSPA-VA. The TH workshop participants formulated the TH issues important to TSPA based on a current understanding of the process-level models and other project experimental data at the time of the abstraction and testing workshop. The resulting list of key issues is given in Section 3.3. This section also includes an overview description of the analysis plans and subsequent work resulting from the TH workshop. Section 3.4 describes the approach and implementation of the TH activities for the VA and provides a detailed discussion of the assumptions applied to the analyses used in support of TSPA-VA. It also elaborates on the supporting analyses that allowed the TH modeling teams to make certain decisions and/or assumptions with regard to development of the TSPA-VA base case. Section 3.5 describes the development of the TH base case for input into TSPA-VA. It describes in detail the development of the required inputs to TH models: thermal and hydrologic property sets, climate states, properties of the engineered materials in the drift, and the reference repository design specifications. Additionally, this section describes the TH multiscale modeling and abstraction method. Finally, this section concludes with the results of the base-case simulations as well as the interpretation of results. Section 3.6 indicates the sensitivity studies considered for the TSPA-VA with respect to TH. Section 3.7 is a summary and discussion of the results of the TH base case and sensitivity studies for TSPA-VA. It includes recommendations for the license application analyses. Section 3.8 lists each of the cited references. Figure 3-9 is a high-level flow chart followed by the TH component of TSPA-VA.

Table 3-3 lists the technical-data-information form numbers, data-tracking numbers, and the descriptions of the data used for the base-case calculations and subsequent sensitivity studies for TH. The tables indicate data-tracking numbers for thermal and hydrologic property sets and thermal-loading data applied to mountain-and drift-scale models. Table 3-4, lists information regarding code status and code version number used in the TH analyses. Table 3-5 contains a summary of the figure results produced by the TH component of the TSPA-VA.

3.2 PROCESS MODEL DESCRIPTION AT THE TIME OF THE ABSTRACTION AND TESTING WORKSHOPS

The Yucca Mountain repository will hold radioactive wastes that emit a large amount of heat from radioactive decay. This heat will influence conditions both close to the emplacement drifts (near-field conditions) and away from the drifts (far-field conditions). The thermal disturbance to the mountain will be affected by how much waste is placed, or loaded, within a given repository area. The areal mass loading used in the TSPA-VA is 85 MTU/acre, which will cause a significant disturbance in the repository environment for thousands of years after waste emplacement.

The project's current understanding of the UZ TH processes is not as advanced as the understanding of ambient UZ flow through the mountain at nearly steady state conditions. This includes theory associated with conceptual flow models as well as applicable hydrologic property sets used to predict steady state flow fields. Transient, thermally driven responses have only recently been accounted for in past TSPAs, typically using a simplified format. Futhermore, with the advent of faster computers (which allow for more detailed numerical meshes) and the results of project expert elicitations on TH, the limitations of the restrictive assumptions typically applied to the TH models are becoming more and more apparent. In particular, severe limitations have been identified related to transient flow processes such as condensate shedding, the prediction of thermal refluxing, and fracture and matrix rock interaction.

Additionally, the understanding of UZ TH and its processes continues to expand on an experimental level with the advent of the Exploratory Studies Facility (ESF) thermal-testing program and the results obtained from the large block test (LBT). The thermal-testing program includes the smaller-scale SHT and the larger-scale drift-scale (DST) test (see for example, Sobolik et al. 1996; Francis et al. 1997a; Francis et al. 1997b; Birkholzer and Tsang 1996 and 1997; Buscheck et al. 1996 and 1997b). Rock heat-up and heat driven water flow processes resulting from a planar heat source emplaced directly into the rock of the LBT are shown in Hardin 1998.

Among other things, the thermal-testing program provides an opportunity for process-level conceptual-model validation and provides information on the coupled TH processes occurring as a result of introduction of heat to a geologic setting. This may include the development of dryout zones with the formation of condensate zones and subsequent episodic water movement through fractures. These same tests may be used to assess hydrologic property sets applied during heat-driven processes. For example, the rate of rewetting in the dryout zone (resulting from heat addition) is a function of that material's matrix diffusivity and fracture capillarity. Both the dryout and rewetting processes in the TH models are currently being estimated using hydrologic

properties obtained from drainage experiments. As a result of the hysteretic nature of the drainage/imbibition curves (corresponding to drying/rewetting processes), the rate of rewetting may not be accurately predicted with hydrologic properties obtained from drainage experiments alone. This may be very important in predicting specific TH processes like the extent of the dryout zone as well as the timing and rate of the collapse of the dryout zone.

The property and conceptual flow issues are important because they serve as the backbone for any predictive solution resulting from a TH model analysis. Although at smaller scales and shorter time periods, using the results of actual heater tests applied in the repository host rock allows for conceptual flow model validation exercises. Subsequently, conceptual model validation increases confidence in the flow models we apply at larger scales and for longer time periods. As a result of all of the above, TH models at the scale of the mountain and drift have increased in complexity with increasing attention to detailed processes such as condensate flow processes, repository edge effects, waste package variability at different repository locations, and the development of large-scale gas-phase movements resulting from a thermal perturbation.

The UZ at the Yucca Mountain site contains in situ water and gas within the pores that will react to the heat generated by radioactive waste. In general, the influence of radioactive decay heat includes: (1) vaporization of in situ liquid water, (2) transport of water vapor (primarily) away from the heat source, (3) condensation of water vapor in cooler regions, and (4) condensate flow, driven by gravity and capillary forces. The decay-heat characteristics of the individual waste packages strongly affect the emplacement drift's thermodynamic environment (its temperature and relative humidity, the amount of water that is liquid and steam, and the time histories, or system responses as a function of time, for fluid flow). The resulting thermodynamic conditions contribute to performance of the repository and engineered barrier system by influencing all of the near-field components of the TSPA-VA.

After waste emplacement, thermal energy will flow from the repository by the heat-transfer processes of conduction and convection. Through these processes, there will be movement of water vapor, liquid water (by both ambient percolation and heat-mobilized condensate), and heat. The heat-transfer processes will result in elevated temperatures and drying in both the surrounding host rock and regions well away from the repository itself. The progression of TH processes through time is pictured in Figure 3-1 and Figure 3-2. Thermally related mechanical and chemical processes can also cause permanent changes to the fluid-flow characteristics of the entire mountain (for example, by changing permeability and porosity). As stated in the previous section, coupled mechanical and chemical processes are included in sensitivity studies only.

Thermal-hydrologic processes occur at two important scales: the scale of the emplacement drifts (a few meters to tens of meters) and the scale of the entire mountain (hundreds of meters to thousands of meters).

Thermal-hydrologic processes at the drift scale include waste-package interactions with both each other and the surrounding drift walls and floor. Heat transfer from waste package to waste package and to the emplacement drift walls and floor occurs predominantly by radiation heat transfer for an open emplacement drift. Heat exchange between waste package and drift wall results in elevated rock temperatures and the propagation of a drying front moving away from the emplacement drifts into the mountain. As the rate of heat generated in the repository

decreases with time, the temperatures decrease and water returns to the emplacement drifts. Drift-scale models can be created which can include different waste packages types with differing thermal outputs. Models that contain this level of discretization can be used to determine variability in temperature, relative humidity, and water flow associated with different waste package types. Information from drift-scale processes is used in models of the near-field geochemical environment, waste-package degradation, waste-form degradation and radionuclide mobilization, and transport of radionuclides through the engineered-barrier system (see Figure 3-4 and Figure 3-7).

Thermal-hydrologic processes at the mountain scale include the influence of heat on liquid and gas movement above and below the repository. Heat from all of the waste packages emplaced in each of the repository drifts enters the host rock through the drift walls. A simplifying assumption for models of this type is that the entire repository heat output can be represented as a single smeared heat source over the heated repository footprint (this number may be scaled for lower dimensional models). This assumption is considered adequate since the resistance to heat flow away from the drift wall (and into the rock) is governed by the host rock itself. Therefore, localized differences right at the drift wall that result from variability of waste package heat output are smoothed out as energy is convected and conducted (at a rate dictated by the thermal and hydrologic properties of the host rock) through the geologic medium. Development of large-scale processes such as edge cooling and buoyant gas-phase convection results from models representing the entire repository heat output in a mountain-scale model domain that include unheated rock masses to the east and west of the repository horizon (as in the case of a two-dimensional mountain-scale model). Information from mountain-scale processes is used in models of the near-field geochemical environment (see Figure 3-4 and Figure 3-7).

Thermal-hydrologic processes at both the drift scale and mountain scale affect fluid flow and transport in the UZ as well; however, for the TSPA-VA we assume that the influence of TH processes is short-lived (see Section 3.5.4.1). In other words, the effect of the thermal disturbance will be over before a significant number of the waste packages have failed so that water seepage into drifts and radionuclide transport from the repository to the water table are not significantly affected by the thermally perturbed water flow fields. Previous models at each scale have been considered by the project in past TH modeling studies.

Previous drift-scale models (both TH and conduction-only) were typically specified as two-or three-dimensional (CRWMS M&O 1994; Buscheck 1996; CRWMS M&O 1995 and 1996c). Two-dimensional drift-scale models are computationally very efficient, but they neglect heat-transfer resistances associated with the finite size of a waste package (CRWMS M&O 1996b, pp. 2.1-12 and 2.1-13). To preserve the areal mass loading in a two-dimensional model, the heat output of a waste package is smeared along the length of the emplacement drift, resulting in a waste package that appears to be infinite in length. Consequently, the waste package heat output is essentially averaged in the model. Three-dimensional models explicitly account for the areal extent (i.e., the true surface area) of the waste package and do not neglect the resistances to heat transfer associated with the surface area of the heat generating source (refer to temperature comparisons made by Bahney 1996 (pp. 29-35), using two-and three-dimensional drift-scale models). Three-dimensional drift-scale models accommodate the potential variability associated with many different waste package types. Three-dimensional models are recommended at this scale, or some method used to correct predictions made by the lower dimensional (2-D) drift-

scale models. Both methods are employed in TSPA-VA. Three-dimensional drift-scale models are used for abstraction testing, while local temperature corrections for different waste package types are applied to the drift-scale models, resulting in perimeter average values.

The obvious drawback of the higher-dimensional drift-scale model is the reduction in computational efficiency. All previous drift-scale models employed by the project use the standard ECM conceptual flow model for heat and fluid flow in fractured porous media. This simplification was necessary to obtain reasonable computational times when performing a TH calculation. As previously stated, TSPA-VA drift-scale TH models employ a dual permeability conceptual flow model assumption, to ensure increased fracture flow of the liquid phase during the condensate-shedding periods and during other processes driven by the thermal perturbation. The applicable model dimensions are one-, two-, and three-dimensional in a system of submodels of varying complexity applied in the TH multiscale modeling and abstraction method (described in detail in Section 3.5.1).

Previous mountain-scale models were typically specified as two-or three-dimensional (Buscheck and Nitao 1993a, 1993b, 1994); Pruess and Tsang 1993; Ho et al. 1996b; Francis et al. 1996). Most of these studies also utilize the ECM conceptual flow model for heat and fluid flow. Ho et al. (1996b, Section 6) considered a two-dimentional mountain-scale simulation, including repository heating, using a dual-permeability model (DKM). This study indicated similar TH results when compared with the ECM simulations, with the notable exception of increased condensate water shedding in the fractures during the repository heat-up and dryout period. That is, disequilibrium processes between fractures and matrix rock allow water to enter the bounding fracture domain and to flow out of the system to cooler regions. Mountain-scale models also predict the gas-phase flow pattern that results from repository heating. Depending on fracture permeability, gas-phase flow may be driven predominantly by pressure gradient (low fracture permeability) or by buoyancy (i.e., density differences) from grid block to grid block (higher fracture permeability). Consequently, fracture properties dictate the mountain-scale prediction of the gas flow field and the evolution of air mass fraction at the repository horizon (see Section 3.5.5.1). In general, TSPA-VA mountain-scale TH models employ a G-ECM conceptual flow assumption. This is considered acceptable since the primary need of the mountain-scale TH model is to predict the gas-phase flow fields and the air mass fraction response at the repository horizon after the emplacement of heat generating wastes. The G-ECM can accurately represent gas-phase flow through an idealized fracture continuum. The model dimension is two dimensional (described in detail in Section 3.5.4).

The preceding descriptions of drift and mountain scales indicate the important physical processes with respect to heat and fluid flow as well as having implications associated with the TH model dimensionality. It is a high-level description indicating processes important to the TH component of the TSPA. Separate and specific components make up each of the high-level processes previously described. For example, heat transfer from waste package to emplacement drift wall requires detailed information related to heat transfer mechanisms that occur resulting from interacting surface properties and other geometric factors. Each of the detailed components making up a process important to TH is described in the following paragraphs.

3.2.1 Thermal-Hydrologic Processes and Parameters

TH processes and parameters considered important for TSPA-VA are discussed in the following sections. The process/issues list was developed by the workshop core teams at the time of the abstraction/testing workshops. It represented the PA understanding of the more important TH process issues and assumptions at the time of the TH workshop (held in January 1997). The resulting analyses plans, developed by the workshop participants, served as the basis for the work incorporated into the TSPA-VA with respect to thermal-hydrology. The important thermal-hydrology issues and processes are presented in four major topic areas: thermal-hydrologic processes and parameters, mountain-scale models, drift-scale models, and coupled processes. It is emphasized that the discussion given herein is in its original format at the time of the workshop. It is included as such so that the reader can clearly see the important issues facing PA at the time of the abstraction and testing workshop. It is intended to establish a method or a means of traceability for the ensuing analyses put forward by the TH component of the viability assessment. The descriptions in this section include both the status of the issue (or TH process) at the time of the workshop as well as how this issue is applied, in general terms, to the current TSPA-VA analyses. The preworkshop descriptions may be written as to how PA may formulate a specific problem. We may also present two or possibly three formulations for a specific component of a problem (for example, how to represent radiation heat transfer in an open emplacement drift). The point of indicating each of the different descriptions as they were understood at the time of the workshop is to guide the reader as to which directions were taken (or may have been taken) when the TH models were developed after the workshop and leading to completion of the TH component of the VA. Regarding a subissue at hand, a very general description of how it is applied in the VA is discussed, with a pointer to a specific section in this chapter that contains a more detailed discussion.

3.2.1.1 Thermal-Hydrologic-Property Distributions

The preworkshop discussion of this subissue was as follows. Required thermal properties of the mountain and EBS included heat capacity, thermal conductivity, and grain density. Thermal properties of the rock mass and engineered components consist of thermal conductivity as a function of liquid saturation. Ranges of wet and dry thermal conductivities of the rock mass can be obtained from regression relations of Rautman (1995, pp. 21, 24, and 25). Rock-grain specific-heat values are available from Nimick and Connolly (1991, p. 39). Particle-grain densities are reported by McKenna and Rautman (1995, pp. 19 and 21) and Nimick and Connolly (1991, p. 34). Thermal properties of crushed backfill have been reported by Ryder et al. (1996, p. 4-42), and correlations reported by Kaviany (1991, pp. 124-126) can be used for other materials comprising the invert. Radiative properties for different materials (and possibly for the waste-package material) can be found in Siegel and Howell (1992, pp. 832-837). New thermal-capacitance (product of the bulk density and specific heat) values have been experimentally measured for various boreholes and rock materials at various depths as a function of temperature (Brodsky et al. 1997, pp. H-3, H-4, and H-9). Thermal-conductivity values have been obtained as well. Additionally, experimental thermal-property values have been obtained from rock samples taken from the ESF.

The lithophysal values for porosity are included in the hand samples taken for thermal conductivity by computing an effective thermal conductivity as shown in Kaviany 1991, p. 126,

using Hadley weighted average. The matrix porosity is subtracted from the total porosity including lithophysal value for porosity. This value is then used as the effective porosity with the intact samples value of used as the effective porosity with the intact samples values of thermal conductivity wet and dry.

Hydrologic properties (fracture and matrix) for the TSPA-VA TH calculations will be taken from the UZ-flow abstraction/testing task. However, it must be noted that variations in these properties with temperature will have to be addressed even if only to argue that these changes are small and that ambient flow properties can be used in the transient problem. The current approach is to ignore temperature dependence (on the hydrologic properties of matrix and fracture) unless proposed otherwise.

Material-property heterogeneity has been considered in the mountain-scale analyses of Ho et al. (1996b, Sections 5 and 6) and Francis et al. (1996, pp. 4-9 through 4-12) for one-, two-, and three-dimensional TH calculations. It was found that material heterogeneity affects the temperature predictions made by the models only in locations in which condensate preferentially moves due to hydrologic property heterogeneity. It directly influences the extent and locations of the condensation zones above and below the repository as well as times and locations for rewetting near the repository. For (laterally) homogeneous-property model domains, dryout and subsequent rewetting tend to be more uniform. For heterogeneous-property model domains, dryout and subsequent rewetting vary along the length of the repository, with some locations rewetting faster than others.

The thermal properties used in the TH component of the viability assessment, TSPA-VA, are provided in detail in TDIF 306664, data tracking number (DTN) SNT05071897001.002. The thermal properties in this package include wet and dry thermal conductivity, heat capacity, and rock grain density. Some of the thermophysical property data used in the models were developed from experimental data (for thermal capacitance and thermal conductivity of variably saturated rock samples) obtained by Brodsky et al. (1997, p. H-3) Other thermal conductivity data were developed from regression relations developed by Rautman (1995, pp. 21, 24, and 25) The thermal data are given in this package for TH models as well as conduction-only models, both used in the TSPA-VA thermal analyses. The thermal property data developed for this TDIF 306664 are not qualified. The hydrologic properties used in the TH models for TSPA-VA are the same property sets used to compute the UZ flow fields and applied directly to the UZ transport calculations (see Tables 2-18 through 2-22 in Chapter 2 of the TSPA-VA Technical Basis Document). The thermal and hydrologic property distributions are for homogeneous layered systems. Therefore, hydrogeologic layer-to-layer property variation is included without any lateral property variation within a layer. The hydrologic property sets are constant in time during a given TH simulation (i.e., mechanical and chemistry alteration to fracture hydrologic properties are neglected—see Section 3.6.8).

3.2.1.2 Fracture/Matrix Interactions (Liquid, Gas, and Heat)

The preworkshop discussion of this subissue follows. Nonequilibrium fracture and matrix rock flow interaction must account for two fundamental mechanisms:

- *Matrix imbibition*—Matrix blocks will imbibe liquid-phase flow from fractures at a finite rate. The ECM assumes that matrix imbibition occurs instantaneously, while the DKM attempts to account for the finite rate of mass transfer between fractures and matrix blocks.

- *Vaporization and vapor flow*—Vaporization in matrix blocks and vapor transport into fractures depend on the temperature and gas-pressure gradients in the matrix blocks. Buscheck and Nitao (1988, pp. 12 and 17) found minor disequilibrium in temperature between fractures and the centers of adjoining matrix blocks. However, depending on size and effective permeability of a matrix block (including matrix and the contribution of small-scale fractures), gas pressure at the center of the block can be considerably greater than in the neighboring fractures. This gas-pressure buildup can suppress the rate of vaporization and the rate at which vapor enters the fractures. The ECM ignores differences between fractures and matrix and consequently does not represent this throttling of advective dryout that may occur in the matrix. The DKM can be calibrated to account for gas-phase disequilibrium between fractures and matrix rock.

Adequately representing the influence of vaporization and vapor flow in matrix blocks is important because it affects the distribution and magnitude of vapor and condensate flow rates in fractures. Phenomena such as buoyant gas-phase convection and the heat-pipe effect may strongly depend on fracture and matrix rock gas-phase flow interactions.

Thermal-hydrologic conditions will promote evaporation and, potentially, precipitation of minerals on fracture surfaces, resulting in a change in how the fracture and matrix rock interact. These THC processes are not currently taken into account in TSPA base-case calculations. Abundant evaporation and subsequent condensation would tend to wet more fracture surface area than under isothermal conditions. This effect could increase the fracture and matrix rock connection area from values used to represent isothermal liquid flow. Physical evidence of the increased wetted area due to condensation is probably unattainable in the allotted time frame, but sensitivity analyses should be done to assess the range of fracture and matrix rock connection areas that significantly influence TH behavior. The suggested approach is to use fracture and matrix-rock connection area as a calibration parameter.

The reduction of fracture and matrix-rock connectivity to simulate channeling of liquid flow and to match borehole saturations (e.g., Altman et al. 1996, pp. 107-108) may not be appropriate for gas and heat flow. Although the wetted portion of a fracture and matrix-rock interface may be very small, the area available for gas and heat flow between the fractures and matrix should be nearly as large as the geometric surface area of the matrix. Past TH simulations comparing the ECM (which, in a sense, has an infinite fracture and matrix-rock connectivity) and the DKM with reduced fracture and matrix-rock connectivity show that the pressures in the matrix for the DKM are slightly higher than for the ECM, presumably because of the reduced connectivity between the fractures and matrix (Ho et al. 1996, pp. 6-10). However, temperatures were very similar between the ECM and DKM and were apparently unaffected by this reduction in fracture and matrix-rock connectivity. The issue of appropriate fracture and matrix-rock connectivity needs to be resolved through sensitivity analyses and any applicable field observations.

The process of calibrating hydrothermal DKM models should take into account both liquid imbibition and vaporization and vapor transport in matrix blocks. In part, this requires the use of simplified models that discretely account for fractures and matrix blocks and sensitivity analyses that examine the dependence on matrix-block size and effective matrix permeability. Determination of the appropriate matrix permeability should address the contribution of small-scale "micro-fractures," which may contribute to vapor flow to the larger fractures that dominate large-scale flow and may also contribute to matrix imbibition of liquid.

In addition to the continuum models discussed above, an alternative conceptual flow model called the Weeps model was used (Wilson et al. 1994, Section 15) in TSPA-1993. The basic assumption in the Weeps model was that matrix flow and fracture and matrix-rock interaction were negligible; all flow was assumed to be divided among discrete fracture-flow channels. The flow in these channels was assumed to be episodic and fast enough that the travel time from repository to water table could be neglected. The strength of the Weeps model lay in its probabilistic calculation to determine how many waste packages were contacted by flow channels. This conceptual model was developed because available process models were not capable of modeling discrete fracture flow. The models unable to account for explicit discrete fracture flow typically include an ECM, and a G-ECM. Both models are typically unable to account for discrete fracture flow in a dryout zone where matrix capillary pressures are high as a result of low liquid saturations.

This subissue is incorporated into this TSPA as follows. The fracture and matrix-rock interaction process applied in the base case viability assessment TH drift-scale model is that specified in the dual permeability modeling approach. Enhanced fracture flow models are applied directly to the drift-scale models used to predict the Engineered Barrier System (EBS) performance attributes. This is to ensure that the wetter conditions (in the drift) associated with fracture flow are characterized in the predictions of the thermodynamic environment of the drift. The dual permeability model uses a constant value or a fluid weighted multiplier on the geometric area conductance term between fracture and matrix rock. The fracture and matrix rock interaction parameter is used to approximate the channeling or finger flow in the fracture network and is applied to liquid flow only. Heat transfer maintains a full conductance area, gas-phase flow nearly a full conductance area. The mountain-scale models used to determine the gas-phase processes driven by heating use an "infinite" conductance between fracture and matrix rock. This is inherent in the assumption governing an equivalent continuum flow model (i.e., equilibrium between fractures and matrix rock). Liquid transport through the fractures in these models is somewhat relaxed for the mountain-scale TH analyses through the application of a G-ECM in which a matrix satiation saturation value is set so as to ensure fracture flow during periods of water movement. The matrix satiates at a value less than fully saturated; therefore, fracture flow occurs in the composite material at lower matrix saturations. The details of each model type are given in Section 3.4.2.

3.2.1.3 Vapor Diffusion (Enhanced or Not)

The preworkshop discussion of this subissue follows. Enhanced vapor diffusion has been postulated to augment the apparent diffusion of condensable gases (e.g., water vapor) through evaporation and condensation mechanisms at the pore scale. Several previous TH models of the potential repository have assumed this behavior (e.g., Pruess and Tsang 1993), primarily because

of its convenient formulation. Under this assumption, the product of the tortuosity coefficient, porosity, and gas saturation are on the order of one, yielding gas-phase diffusion in the porous medium that is equivalent to gas-phase diffusion in free space. (This formulation predicts vapor diffusion even for fully saturated conditions.) Although experiments in the soil-science literature have supported this theory, no information is available for consolidated rock. Sensitivity analyses should be performed comparing TH simulations with varying degrees of vapor-diffusion enhancement to determine its importance in TSPA calculations. Another consideration is that if enhanced vapor diffusion is not to be used, an appropriate model for the tortuosity coefficient must be developed.

An explanation of the implementation of this subissue into the TH component of the TSPA-VA follows. A lack of data for a tortuosity coefficient for consolidated rock necessitated the use of vapor diffusion models from the soil science literature. This diffusive transfer term is developed in TDIF 306664, DTN SNT05071897001.002. The developed data for the vapor diffusion parameter are nonqualified.

3.2.1.4 Thermal-Hydrologic Flow Regimes

The preworkshop discussion of this subissue follows. There are three major TH flow regimes with respect to vaporization and rock dryout (Buscheck and Nitao 1995, pp. 17-19; Buscheck 1996). The three regimes are primarily affected by the fracture-permeability distribution:

- *Throttled, nonbuoyant*—Roughly, bulk permeabilities below 1 millidarcy ($k_b < 10^{-15}$ m^2). Permeability is low enough to significantly throttle the rate of boiling-driven advective rock dryout. Throttling can also occur if the matrix blocks are sufficiently large and their effective permeability is sufficiently small.

- *Unthrottled, nonbuoyant* ($10^{-15} < k_b < 1 \times 10^{-12}$ m^2)—Permeability high enough not to throttle boiling-driven advective rock dryout, but not high enough for buoyant gas-phase convection to dominate vapor flow.

Matrix blocks must be small enough not to throttle the rate of vapor flow into the large-scale connected fracture network.

- *Unthrottled, buoyant* ($k_b \geq 1 \times 10^{-12}$ m^2)—Permeability is high enough to allow buoyant gas-phase convection to dominate vapor flow. For $k_b > 40 \times 10^{-12}$ m^2, buoyant gas-phase convection dominates the heat flow as well.

If matrix blocks are large enough, vapor flow from the matrix blocks to the large-scale connected fracture network can be throttled, thereby reducing the magnitude of buoyant gas-phase convection. This is a gridblock-scale issue.

An understanding of these TH flow regimes is important to keep in mind when developing and calibrating DKM models and when upscaling and developing distributions for hydrologic properties.

The gas-phase flow fields discussed in the preceding subsections are important to the redistribution of both moisture and heat. If a range of fracture properties is to be considered in TSPA calculations (to be determined in conjunction with the UZ-flow abstraction/testing task), and mountain-scale TH is not included in the TSPA-VA abstracted flow model, then sensitivity studies can be used to determine the range of flow fields that may result from the choice(s) of fracture properties used. The determined flow-field variability could then be used to modify the assumed percolation rates (or other form of simplification/abstraction) to partially account for the thermal effects not explicitly included in the UZ-flow calculations. (To put it another way, a response surface could be developed that gives percolation flux over time to be used in isothermal flow calculations as a function of infiltration, bulk permeability, and possibly other quantities.)

An explanation of the implementation of this subissue into the TH component of the TSPA-VA follows. For TH, we are primarily concerned with the units in which the heat source is directly emplaced. For the current VA repository design, this results in repository placement into the Middle Nonlithophysal (Tptpmn), Lower Lithophysal (Tptpll), and the Lower Nonlithophysal (Tptpln) units. Within each of these units, the bulk fracture permeabilities exhibit characteristics of the unthrottled, buoyant ($k_b \geq 1 \times 10^{-12}$ m^2) regime. In this case, density differences from model cell to model cell transport both mass and heat away from the repository. The thermal perturbation of the UZ flow field (liquid flow below the repository horizon) is determined to be short-lived (see Section 3.5.5). Therefore, it is neglected in the transport calculations through the UZ.

3.2.2 Mountain-Scale Models

3.2.2.1 Repository Design and Thermal Source

The preworkshop discussion of this subissue follows. Repository design criteria will be established in the spring of 1997. These criteria should include waste-package and drift dimensions, waste-package spacing, drift spacing, initial repository thermal load, and areal extent of the repository. In their simplest form, mountain-scale models require only the average thermal load over time and the areal extent of the repository.

A topic discussed at the TH workshop was whether there are alternative designs that should be analyzed as part of TSPA-VA. Even if the "official" design specifies a single thermal load and emplacement pattern, it may be worthwhile for TSPA to perform comparisons with one or more alternatives, such as lower or higher thermal loads, "line" loading, engineered capillary barriers, or natural ventilation.

Waste-stream variability can be included in mountain-scale calculations to a certain extent by varying source thermal outputs from cell to cell, but such variations are more appropriately considered in drift-scale calculations. If the repository design should call for large-scale thermal-loading variations (e.g., by segregating the glass waste or cooler spent fuel in one section of the repository), sensitivity studies can be used to establish possible wet zones in the repository as a result of nonuniform loading of the waste. Waste-stream variability could require the use of repository-scale models that fall between drift-scale and mountain-scale models, or it could be

necessary to "nest" drift-scale models at various repository locations into a repository-scale or mountain-scale model that accounts for the repository-scale condensate redistribution.

An explanation of the implementation of this subissue into the TH component of the TSPA-VA follows. The thermal load used in the two-dimentional mountain-scale TH models is spatially uniform and is made up of the heat decay curves from the expected quantity of CSNF, defense HLW, and DOE SNF to be emplaced in the repository. The two-dimensional mountain-scale model assumes that the drifts are sealed, although sensitivity studies are performed that investigate open drifts from which gas can enter or exit the repository. Another sensitivity study investigates the delayed emplacement of the waste into the repository (i.e., interim storage outside of the mountain or ventilation of nonbackfilled drifts for some time after waste emplacement). Higher or lower thermal loads are not considered for the TSPA-VA but lower thermal loads are being addressed in Environmental Impact Statement (EIS) activities. The details of "line" loading can be found in Section 3.6.4. Waste stream variability was not included in TSPA-VA mountain-scale activities.

3.2.2.2 Dimensionality of the Problem

The preworkshop discussion of this subissue follows. It is possible that computational limitations and the large number of calculations required will preclude running a full three-dimensional TH model to describe the mountain and repository. Therefore, we may need to reduce the model dimensionality for the TSPA-VA TH calculations. One drawback of reduced-dimension X-Z models is that a semi-infinite or infinite repository is implied. For a model reduction from three-dimensions to two-dimensions, the repository becomes semi-infinite in extent. For a reduction from three-dimensions to one-dimension, the repository becomes infinite in extent. Radial "R-Z" models can reduce the problem to a two-dimensional representation and still maintain a finite heat source; however, tilting of stratigraphy, the infiltration rates, and other geologic features cannot be modeled with this type of model. One benefit of reduction in model dimensionality is that it allows for many calculations to be run in a timely manner. Uncertainties in the models and model parameters require that many calculations be performed in order to establish uncertainty in the repository performance. To be able to take advantage of reduced-dimensionality calculations, however, it must be satisfactorily shown that a reduction in model dimension does not significantly change the results (specifically, it is important that radiation-dose predictions not be underestimated significantly).

It may be feasible to argue that dimensionality reduction results in a conservative estimate (i.e., tending to overestimate peak doses) of how repository heat will affect the far-field transport of radionuclides. One-dimensional mountain-scale TH models result in slightly higher temperatures and larger (vertical extent) dryout zones (or at later times, drier-than-ambient regions). This trend persists for more than 10,000 years after waste emplacement (Ho et al. 1996, pp. 6-8 to 6-10). This effect is considered to be nonconservative (that is, tending to underpredict peak radiation doses), directly resulting from the infinite extent of the modeled repository. The mass flow of liquid in a one-dimensional model is directed vertically downward at all times, with no lateral flow allowed. Vertical flow may or may not be conservative, but one result of constraining flow to be vertical is to predict an artificially large gas-pressure buildup beneath the repository (the water table is a barrier to gas flow and gas is not allowed to escape sideways). This artificially increases upward vapor flow, and tends to mimic the effects of

mountain-scale buoyant gas-phase convection. If one-dimensional results can be shown to be reasonably close to correct, or conservative, the reduction of the mountain-scale TH models to one dimension may be justified for TSPA-VA calculations. Sensitivity studies can be performed for a limited number of three-dimensional mountain-scale runs in order to make comparisons to two-dimensional and one-dimensional runs.

An explanation of the implementation of this subissue into the TH component of the TSPA-VA follows. A two-dimensional mountain-scale model is used for all mountain-scale TH calculations. It was not necessary to reduce the mountain-scale TH models down to one dimension. Detailed three-dimensional mountain-scale TH models remain beyond the capability of current computational capability. A comparison of three-dimensional mountain-scale ECM simulation results (Francis et al. 1996, Chapter 4) and two-dimensional mountain-scale ECM simulation results (Ho et al. 1996, Chapter 5) showed similar results.

3.2.2.3 Boundary Conditions

The preworkshop discussion of this subissue follows. Constant temperature (Sass et al. 1988, Figure 10), pressure, and relative-humidity (or air-mass-fraction) boundary conditions (at the ground surface) may be used in TSPA calculations. Constant property boundary conditions may also be applied at the water table. The infiltration rates applied at the ground surface boundary in the models used for TSPA-VA TH simulations must be consistent with ranges determined in the UZ-flow abstraction/testing task. Episodic infiltration events may be considered in addition to steady infiltration boundaries if deemed necessary. Recent measurements indicate a mean annual atmospheric relative humidity of 37.5%. The "net infiltration" is the surface infiltration minus evaporation, giving a net percolation flux in the mountain. The atmospheric temperature and relative humidity presumably should change with climate along with changes to the infiltration rate.

The lateral boundaries for mountain-scale models should be far enough from the domain of interest that behavior of the thermal perturbation is not affected by them. Constant-temperature or adiabatic no-flow conditions can then be used. Sensitivity analyses similar to those performed by Ho et al. (1996b, pp. 5-15 and 5-16) can be performed to determine the validity of these assumptions by applying adiabatic and constant-temperature lateral boundaries as two extreme bounding conditions.

An explanation of the implementation of this subissue into the TH component of the TSPA-VA follows. The two-dimensional mountain-scale model used constant temperature and pressure boundaries at the ground surface and at the water table boundaries and no-flux boundary conditions at the lateral boundaries. The relative humidity was set at 100% and the infiltration rate was specified at the surface, which yielded the proper percolation flux into the mountain. Sensitivity studies were performed to investigate the impact of using constant-temperature boundary conditions at the water table, adding the high permeability Solitario Canyon and Ghost Dance faults to the simulation domain, and raising the water table 80 meters during a climate change from a dry climate to a wet climate.

3.2.2.4 Perched Water Below the Repository

The preworkshop discussion of this subissue follows. Perched water can act as a source of water that is mobilized by heat. The impact of perched water on the TH response of the potential repository can be assessed through sensitivity studies using existing TH process models by adding a SZ beneath the repository (above the water table) with a matrix permeability of zero (or near zero) to simulate a perched water body. Note that if a calibrated UZ-flow model is used as a starting point for the TH calculations, perched water will automatically be included, but it requires the use of the three-dimensional site-scale model for TH analyses.

Another issue with regard to perched water is that thermal-chemical or thermal-mechanical processes may cause increases or decreases in bulk permeability that lead to decreases or increases in the extent of perching. For example, alteration of glasses could cause plugging of fractures; dissolution of existing fracture fillings at elevated temperatures could cause unplugging of fractures; and thermal-mechanical stresses could cause creation of new fractures or even movement on the block-bounding faults.

An explanation of the implementation of this subissue into the TH component of the TSPA-VA follows. The effect of the thermal perturbation on perched water was not included in TSPA-VA. The east-west two-dimensional mountain-scale TH simulation domain was located through the center of the repository and did not include any perched water. The effect of the thermal perturbation (ignoring permanent chemical or mechanical changes to the host rock) on the water flow fields in the UZ is not expected to last more than 1,000 to 5,000 years (see Section 3.5.4.1). Consequently, although the presence of perched water has been shown to be important to UZ flow and transport (see Section 2.5.1.1 in Chapter 2 of the TSPA-VA Technical Basis Document), the overall effect of TH on the UZ flow is thought to be a short-lived phenomenon and is, therefore, not included in TSPA-VA.

3.2.3 Drift-Scale Models

3.2.3.1 EBS-Design Issues and Heat-Source Variability

The preworkshop discussion of this subissue follows. The discussion in Section 3.2.2.1 on design alternatives applies to drift-scale models as well. In addition, at the drift scale, waste-package variability is an issue.

Variability of heat output from waste package to waste package could be important to repository performance because of the potential for shedding of thermally mobilized water onto the cooler packages. Three-dimensional drift-scale calculations (Buscheck 1996a, Section 1.10; Buscheck et al. 1997b) show that variability in waste-package heat output can cause large variabilities in dryout, rewetting, and liquid-phase flux along drifts. Consideration of this effect requires a multi-package drift-scale model in order to include both "hot" and "cold" waste packages in the same calculation. Such a model must necessarily be three dimensional. A sensitivity study is needed to determine whether waste-package variability should be included in TSPA-VA calculations.

An explanation of the implementation of this subissue into the TH component of the TSPA-VA follows. A three-dimensional drift-scale sub-model in the TH multiscale modeling and abstraction method includes placement of both the hot and cold waste packages. It contains representative numbers of each waste package type emplaced in the repository, including commercial spent fuel and additional wastes (see Section 3.5.3).

3.2.3.2 Dimensionality of the Problem

The preworkshop discussion of this subissue follows. As in the case of mountain-scale modeling, a full three-dimensional representation of the waste package and drift environment would be desirable. In fact, drift-scale calculations are much more adversely affected by reduction in model dimension than are mountain-scale calculations. The reduction from a three-dimensional to a two-dimensional drift-scale TH model neglects heat-transfer processes from finite-sized waste packages to the drift wall (M&O 1996b, pp. 2.1-11 to 2.1-16). The reduction of a three-dimensional drift-scale model to a two-dimensional one is accompanied by the assumption that a waste package is infinite in extent in the direction along the length of the drift. From a heat-transfer point of view, this is equivalent to reducing the surface-area resistance to heat transfer from the waste package to the drift wall, resulting in lower waste-package temperatures. The lower temperatures will cause higher relative humidity in the drift. In addition, for a cooler drift, the dryout zone will not advance as far from the drift for as long (also serving to increase the relative humidity in the drift).

The prediction of a lower waste-package temperature is probably nonconservative from a waste-form-degradation point of view (e.g., resulting in lower oxidation rates). In contrast, the higher relative humidities predicted by two-dimensional models are probably conservative for waste-package-degradation models. If low-thermal-conductivity backfill is emplaced (e.g., crushed tuff), the temperatures predicted by two-dimensional and three-dimensional models (M&O 1996b, pp. 2.1-11 to 2.1-16; M&O, 1996c, pp. 3-4 to 3-11) just after backfilling can differ by 100°C or more. This difference in peak waste-package temperature can result in substantially different performance, not just in predictions of cladding failure, but also for waste-package corrosion and for oxidation of fuel in waste packages that fail early.

An explanation of the implementation of this subissue into the TH component of the TSPA-VA follows. Various model scales are employed by the TH multiscale modeling and abstraction method (see Section 3.5.1 for a detailed description of the multiscale abstraction method). Two-dimensional, drift-scale TH calculations are used to obtain average temperature and relative humidity characteristics because of waste package heating at the emplacement drift wall. The predictions made by the two-dimensional (drift-scale) models are corrected at the waste-package surface and emplacement drift wall by a three-dimensional drift-scale thermal model. The three-dimensional model allows for finite-sized waste packages with different heat outputs. The correction is made so that the localized heating differences resulting from different thermal outputs from package to package can be captured and incorporated into the calculation of the average characteristics computed by the lower dimensional models. The net effect is that the appropriate heat flow from an actual-sized waste package is accounted for within the combination of the two drift-scale models.

3.2.3.3 Boundary Conditions and Coupling to Mountain-Scale Models

The preworkshop discussion of this subissue follows. In their current forms, drift-scale models tend to extend from the ground surface down to the top of the water table. The lateral width tends to be that of the symmetry pillar spacing, resulting in a tall, very skinny model domain. This model feature can result in volume elements both above and below the drift, with unfavorable aspect ratios. This numerical problem can be eliminated by coupling the drift-scale models to mountain-scale models.

Mountain-scale analyses can provide time-varying boundary conditions for the drift-scale models. This would allow one to reduce the drift-scale model domain to regions specifically including the near field only. As a direct result of this extent reduction, some grid refinement could be performed in the drift itself and around the waste packages. This would help resolve (numerically) convective heat-transport processes inside the drift. The time-varying boundary conditions (taken from a mountain-scale simulation at a given thermal load) can be implemented into a drift-scale calculation in much the same way that the time-varying heat source is introduced in most flow codes. The problem of determining the appropriate volume-element sizes (assigned to the mountain-scale models) to provide time-dependent inputs to drift-scale models such as temperature, liquid saturation, gas-phase pressure, and liquid mass flow would need to be resolved in a computationally efficient manner.

An explanation of the implementation of this subissue into the TH component of the TSPA-VA follows. Coupling between drift-scale and mountain-scale models, through the use of time-dependent boundary condition inputs to the drift-scale models, is not implemented in the VA as described above. With the use of the TH multiscale modeling and abstraction method (see Section 3.5.1), the drift-scale model results are implicitly coupled to mountain-scale model results through a derived temperature relationship between models. The temperature relationship is used to correlate an average temperature for the repository host rock as computed by a smeared heat source, three-dimensional, mountain-scale, thermal model to the averaged temperature of the drift wall predicted by a line-averaged (for example, two-dimensional) heat source, drift-scale, TH model. The correlation is required since the average temperature of the repository host rock is computed from a conduction-only mountain-scale model and hence must be corrected for the fluid components of the system. The TH model used in the temperature correlation is a two-dimensional drift-scale model with sufficient discretization at the waste package and emplacement drift wall to resolve the heat-driven processes that occur in and around the drift after waste emplacement. Since it is two-dimensional, further grid refinement is allowable. The two-dimensional drift-scale model contains top and bottom boundary conditions at the ground surface and the water table, respectively. This is a requirement since these are the locations in the mountain at which boundary conditions are assumed to be known with respect to time (for heating periods of hundreds of thousands of years). Lateral boundary conditions are periodic and no-flow to heat and mass transfer. This assumption represents downward flow (vertical) but may underestimate heat-driven lateral flow (horizontal), in particular at repository edge locations. (Repository edge locations are discussed in an upcoming discussion.) The net result of this process is an approximate drift-wall temperature from a mountain-scale model with a finely resolved, line-averaged heat source, which can be computed at different locations throughout the repository. It includes the hydrology component of the system. This is an example of an abstracted model.

3.2.3.4 Heat and Mass Transfer in the Drifts

The preworkshop discussion of this subissue follows. Three modes of heat transfer will occur in the drift environment: radiation, convection, and conduction. For open drifts, all three modes are present, with radiation as the dominant mode of heat transfer. For backfilled drifts, conduction and convection heat transfer are both present, but radiation no longer dominates the flow of heat from the waste package. Mass transfer (i.e., a gas-phase velocity) occurs inside an open drift as a result of gas flow as well as from moisture migration from the drift walls during drying (Ho and Francis 1996a, pp. 5 and 6). An important issue for open drifts is how best to model the fluid advection. Should this be done at all using a porous-medium flow code? What effective permeability should be assigned to an open drift to model mass (and heat) flow in an open drift if one chooses to use a porous-medium flow code? It may be necessary to neglect convection processes in an open drift altogether and assume that the heat transfer is radiation-dominated (possibly using an effective thermal conductivity if radiation is not implemented rigorously). These assumptions can be checked against empirical data, but it is possible that they are nonconservative (because of convective moisture movement) for only a short time after waste emplacement. For backfilled drifts, gas-phase convection will be calculated properly by porous-medium codes provided that the spatial and temporal discretization is adequate.

An explanation of the implementation of this subissue into the TH component of the TSPA-VA follows. Radiation heat transfer is explicitly represented between all surfaces in the emplacement drift. The base-case repository design is for an open drift (for example, no backfill material). In this case, radiation heat transfer occurs between package-to-package, package-to-floor, package-to-emplacement drift wall, floor-to-wall, and wall-to-wall. For two-dimensional drift-scale models, there is no package-to-package radiative connection. For an open emplacement drift, radiation is the dominant mode of heat transport from the waste package surface to the emplacement drift wall. Although not a dominant mode of heat transfer in an open drift when compared to radiation heat transfer, convective heat flow (and hence mass transfer) along the axis of the emplacement drift is included in such a way that the gas-phase pressure predicted by the model will not increase as a result of throttling of gas-phase flow.

3.2.3.5 "Center" vs. "Edge" Thermal-Hydrologic Response

The preworkshop discussion of this subissue follows. Coupling mountain-scale models to drift-scale models may provide for the most natural means of making repository-edge and -center waste-package temperature, relative-humidity, and water-seepage predictions. This can be accomplished by selecting the output from a mountain-scale model at center or edge locations and providing time-dependent boundary conditions to a reduced-in-extent drift-scale model domain. If it is found that coupling is not numerically or physically feasible, the use of a "unit cell" model can still be applied as a center representation, but an alternative representation is required for modeling waste packages near the edge of the repository. (A problem with the unit-cell approach is similar to that mentioned earlier for one-dimensional mountain-scale models: they can predict an artificially large gas-pressure buildup below the repository and artificially increased upward vapor flow. These effects can result in too much condensate buildup above the repository and drainage of condensate into the repository.)

One method may be to approximate the edge with a multiple-drift (how many drifts would be necessary?) model linked to a semi-analytical conduction solution. One method would be to use the Vinsome and Westerveld solution (Pruess 1991, pp. 35-37), in the unloaded rock mass coupled to a multiple-drift-scale model. This would approximate the flow of heat from the end drift(s) into the surrounding host rock not containing drifts. For full-extent three-dimensional drift-scale models (from the ground surface down to the top of the water table), this potential solution technique at the repository edge may be very computationally demanding.

In CRWMS M&O (1995, p. 4-13), a scaling concept was introduced in order to approximate edge behavior. It was hypothesized that the edge response was identical to center response, but at a lower thermal load. In order to find the new thermal load, two-dimensional and one-dimensional mountain-scale models were used to match temperatures, liquid saturations, and pressures. When the matching solution was obtained (by trial and error), the reduced thermal load was used in the center-cell representation. (Note: for the implementation of TH to TSPA-VA, this method is used in the drift-scale models developed to test the TH multiscale modeling and abstraction method. It is not used to generate the base case results for repository edge located waste packages. An alternative approach for edge response is discussed below and in more detail in Section 3.5.4.2).

A hybrid drift-scale/mountain-scale abstraction approach is described in Section 1.10.6 of Buscheck (1996). This approach uses a mountain-scale model to predict average TH conditions in the rock at a selected repository location, superposed with the results of a drift-scale multiple-waste-package model.

An explanation of the implementation of this subissue into the TH component of the TSPA-VA follows. As discussed in Section 3.2.3.3, all repository locations (center and edge locations among others) can be analyzed with the implicit coupling between drift-scale and mountain-scale models as described in the TH multiscale modeling and abstraction method described in Section 3.5.1. The net result of this process is an abstracted mountain-scale model with a line-averaged heat source at any location within the repository (recall that this abstracted model reproduces average temperature and relative humidity at the emplacement drift wall). This includes the repository edge locations as well.

3.2.3.6 Seepage Into Drifts

The preworkshop discussion of this subissue follows. Flow channeling and seepage into drifts and onto waste packages may be altered by the presence of hot waste packages and the drying of the host rock near the drifts. The extent and duration of drying and its influence on flow channeling and seepage will depend on the chosen process model. Current thoughts are to combine process models using equivalent-continuum or dual-permeability models with Weeps modeling to abstract the effects of the thermal perturbation on flow channeling and seepage. There may be significant evaporation of water penetrating hot rock and seeping into a heated drift, resulting in much less water actually contacting waste packages (Nitao and Bradford 1997). At the same time, however, the evaporating seepage might contribute to raising the humidity in the drift locally.

An explanation of the implementation of this subissue into the TH component of the TSPA-VA follows. A sensitivity study using the seepage flow model developed for the UZ flow model incorporates thermal reflux values in the host rock three meters above the crown of the drift for three different waste package types (see Section 3.6.5).

3.2.4 Coupled Processes

3.2.4.1 Thermal-Hydrologic-Chemical

The preworkshop discussion of this subissue follows. Chemical effects in response to a high thermal load in the repository can permanently alter material hydrologic properties. Phase-change processes occurring around the dryout zone will cause chemical precipitation-dissolution and thus alterations to fracture and matrix properties such as permeability and porosity. These changes will then influence the resultant flow fields not only while the thermal process is active but afterward. In addition to possibly significant changes around emplacement drifts, hydrothermal alteration of glasses in the Paintbrush Tuff nonwelded tuff, Topopah Springs basal vitrophyre, and Calico Hills nonwelded geohydrologic units could cause significant changes in post-thermal mountain-scale water flow.

An explanation of the implementation of this subissue into the TH component of the TSPA-VA follows. Preliminary TH-chemical modeling (Hardin 1998, pp. 5-57 through 5-67) considered silica within the fracture system in the UZ. This fully coupled TH-chemical study was at the drift scale. The study included reactions for silica-cristobalite-quartz in the fracture and matrix system. Changes in fracture and matrix porosity (which also affect fracture permeability) caused by mineral dissolution and precipitation were calculated. Waste-package temperature and relative-humidity time histories were not greatly affected by the reactive-transport processes included in the simulation, even though mineral cap formation above the drifts (Hardin 1998, Figure 5-35). However, the effects on seepage flow into a drift because of a mineral cap formation above the drift have not been fully investigated (see Section 3.6.8).

3.2.4.2 Thermal-Hydrologic-Mechanical

The preworkshop discussion of this subissue follows. Thermal stresses can cause material-property alterations in regions of compression and tension. For an 80-kW/acre repository load and a given initial stress state, significant fracture-aperture alterations occur as early as 25 years after waste emplacement (Mack et al. 1989, Figure 3-15). Mack et al. (1989) found that thermal-mechanical effects caused fracture apertures to decrease by a factor of two in regions near the repository. Regions of tension occur both above and below the repository horizon. In these regions, fracture apertures were found to increase by a factor of two. As time progresses, the regions of tension decrease above and below the drifts as the region of compression grows. The region of compression can even approach the ground surface (in about 500 years in the calculations of Mack et al. 1989, Section 3, Figure 3-19).

Fracture-aperture closure might limit the development of buoyancy-driven gas-phase transport near the drift. This effect could limit the growth and extent of the dryout zone surrounding the drift. Temperature predictions might also change if gas-phase convection becomes limited by

reduction in fracture apertures. (According to the cubic law, a reduction in fracture aperture by a factor of two corresponds to a decrease in bulk permeability by a factor of eight.)

In addition to aperture openings and closings, thermal-mechanical stresses will induce new fractures and movement on joints and possibly even on faults. Such changes are irreversible, so the system would not return to the initial (undisturbed) ambient state.

Limited process-level TH calculations can be performed assuming changes in fracture permeability and porosity caused by these processes, starting at different times after waste emplacement, to determine a range of possible responses in the gas-phase flow field. The overall effect that THM coupling could have on the predicted flow fields could be estimated from such calculations.

The implementation of this subissue into the TH component of the TSPA-VA the follows. It is treated as a sensitivity study to determine impact on predicted flow fields. Preliminary THM modeling (Ho and Francis 1998) has indicated that the liquid-phase flow fields for a one-dimensional, dual-permeability model at the mountain scale are essentially unaffected by increases or decreases of approximately ten times the value used for the permeability in vertical fractures because of thermal loading and subsequent thermal stresses. Based on this modeling, THM alteration of the flow field below the repository is considered negligible (see Section 3.6.8).

3.2.4.3 Drift Collapse and Its Effects on Temperature, Relative Humidity, and Seepage Into the Drift

The pre-workshop discussion of this subissue follows. If emplacement drifts are left open, without an engineered backfill, then they could be vulnerable to collapse as a result of thermal-mechanical or seismic stresses. Among the possible effects of drift collapse are (1) direct failure of containers, (2) enhanced container corrosion because of container damage or because of contact with rubble, (3) increase of container temperature as a result of increased thermal insulation, and (4) greater thermal isolation of waste packages from each other, resulting in more persistent temperature and relative-humidity variations along the drift. Effects (3) and (4) will be studied in the TH models developed for TSPA.

To our knowledge, the only consideration of this effect has been by Gauthier et al. (1996 p. 4), who showed that there could be a significant increase in waste-package temperature because of drift collapse. The amount of increase depends on the time of collapse and on the thermal conductivity of the rockfall rubble. Unfortunately, neither of these quantities is known, so there is a great deal of uncertainty about the magnitude of the effect. If no further information can be found, "expert judgement" will have to be used to develop ranges for these variables. With the assumptions made by Gauthier et al. (1996), the thermal effects of rockfall were not found to have a great effect on repository performance.

An explanation of the implementation of this subissue into the TH component of the TSPA-VA follows. A sensitivity study is performed using a three-dimensional drift-scale TH model. This model is necessary in order to obtain information concerning the response of the engineered barrier system when different waste-package types are exposed to a specific rockfall even. For

the TH component of the VA, a preliminary rockfall analysis, the focus is on the resulting thermal (temperature) and hydrologic (liquid saturation and relative humidity) environment at the waste package resulting from a rubblized zone surrounding a heated waste container. This analysis does not consider any damage that may occur (if any) to the waste package itself as a result of the rockfall. For this sensitivity analysis, rockfall is assumed to occur uniformly at 1,000 years after the emplacement of waste. Assumptions are made regarding the rock properties upon collapse into an open drift. Different heat and fluid flow properties are assumed to determine the relative influence of different heat transfer modes in the rubblized zone (see Section 3.6.6).

3.3 ISSUES ASSOCIATED WITH THE THERMAL-HYDROLOGY COMPONENT OF THE TSPA-VA

The previous section in this chapter provided a description of the process-level model issues associated with the TH component of the TSPA-VA. It described models of different scales, dimensions, and flow-process-oriented assumptions used to develop data associated with the performance attributes of the engineered barrier system and the entire mountain during the thermal perturbation. The TH component of the TSPA provides information for the "altered" zone of the mountain. This includes both near-field and far-field considerations because waste decay heat impacts the mountain not only in the near-field but from the ground surface to below the water table. The previous section in this chapter described approaches that could have been followed for the current TSPA. Also, it described, in general terms, how particular issues raised at the workshop were implemented in the TSPA-VA. If a workshop issue was not implemented, a discussion as to why and what its impacts may be was given. The current section describes the prioritization of the TH issues (given in Section 3.2) and how the key issues were obtained with respect to the specified performance criteria associated with the near-field environment.

Previous TSPAs (Wilson et al. 1993, Section 10; CRWMS M&O 1995, Sections 4 and 9) have included the influence of thermal effects on predictions of radionuclide releases from the repository and subsequent doses to the public. Many of the model assumptions and simplifications in previous TSPA thermal analyses have been improved for the TSPA-VA. These improvements include assumptions related to dimensionality (that is, modeling in one, two, or three dimensions) and conceptual flow models for heat and mass transfer. In addition, there is a considerable amount of recently acquired thermal and hydrologic data that has been used in the TSPA-VA.

In order to accomplish similar improvements for the viability assessment, the project instituted abstraction and testing workshops to address any outstanding or new issues related to each of the process-level models used in support of TSPA. Before the workshop, performance assessment personnel were tasked to develop a plan for the viability assessment TSPA that would include the most current information available to the project at the time of the workshops. A process-level description of the TH assumptions and physical processes was based on our understanding of the governing TH processes and parameters at the onset of the abstraction and testing workshop. The overriding goal of the TH abstraction and testing workshop was to determine the manner in which PA may develop valid, defensible, models and abstraction processes using the most complete and current information available to the project.

Examples included the use of recent project experimental data describing the thermophysical properties of the rocks of Yucca Mountain, heating results obtained directly from the Exploratory Studies Facility thermal testing program (e.g., single-heater test), and the recommendations of the TH Modeling and Testing Program Peer Review (YMSCP 1996, pp. 75-81). Also, new information related to the infiltration rate at Yucca Mountain required further consideration by the TH modelers. In past TH models, infiltration rates ranged from 0 to about 0.3 mm/year. Current project data indicate infiltration rates more on the order of 1 to 10 mm/year. Climate changes will result in even higher infiltration rates. The importance of infiltration rate on TH model predictions of temperature and dryout has already been established (Ho 1997; Hardin 1998).

A key effort in formulating the TSPA-VA models was the workshop convened by the performance-assessment group in January 1997 (CRWMS M&O 1997a). Attendees included personnel specializing in site characterization, repository subsurface design, and waste-package design, as well as an array of performance-assessment analysts who model the total repository system and individual processes. Workshop participants represented many components within the project to ensure consistency among the various groups and the best use of current data sources.

Workshop participants developed a list of issues and prioritized them based on criteria for long-term repository performance. The criteria provided a basis for quantifying long-term performance of a potential geologic repository. The prioritization criteria related the issues to the thermodynamic environment in the drift (required input to near-field and EBS models) and to far-field flow below the repository horizon. The criteria were:

Does the TH process/issue affect the magnitude, spatial distribution, or temporal variation of:

A. Waste package temperature
B. Relative humidity around a waste package
C. Liquid water flow rate into the drift environment and onto a waste package
D. Aqueous flow from the repository to the SZ.

The key issues important to TH resulted from consideration of each issue specified in the context of criteria (A through D) listed above. The criteria are all specific performance measures that have important contributions to post-closure repository performance assessment.

The issues and processes were categorized as follows: TH processes and parameters, mountain-scale models, drift-scale models, and important coupled processes. The most important key issues that resulted from the four main workshop categories included the following:

- What models should be used to depict the interactions between fractures and matrix rock?

- How should fracture properties and TH processes be modified for upscaling (that is, accounting for differences between small-scale experiments and observations applied to larger-scale features)?

- How important are the trade-offs among using one-dimensional, two-dimensional, and three-dimensional modeling for the mountain-scale models?

- How important is the dual-permeability model, which uses different permeability values for fractures and matrix rock, at the mountain scale?

- Will variability of heat output among waste packages allow for condensate shedding onto cooler packages?

- Is it necessary to develop drift-scale models that represent conditions at the repository edge as well as those at the repository center?

- How should water seepage into drifts and onto waste packages during thermal periods be modeled?

The workshop participants determined that conceptual models allowing for more flow through fractures, in particular during the thermal periods (see Figure 3-1), would be the most appropriate for the TSPA-VA. The conceptual models for increased fracture flow are the generalized ECM and the DKM. The latter gives a more physically realistic description of a thermally driven system and ensures consistency with the flow models for the UZ (see Chapter 2 of the TSPA-VA Technical Basis Document). More movement of water through fractures allows condensate or reflux waters, mobilized by heat, to drain through fractures either back to the drifts or between the pillars separating drifts.

Identification of the key issues during the abstraction and testing workshop led to development of the analysis plans, which were used to guide and help build a valid, defensible, TSPA-VA with respect to the TH component of a potential geologic repository. The analysis plans developed during the workshop were based on resolving the key issues. They were a result of discussions and working sessions with the project experts associated with the repository design, site characterization, property measurements, process-level models, and TSPA models. Each of the analysis plans provided the backbone for the ensuing work that TH analyses groups completed in support of the TSPA-VA. The analysis plans resulted in mountain-scale models, drift-scale models, and some preliminary estimates of nonisothermal seepage processes and coupled processes of mechanics and chemistry. A detailed description of the analysis plans is in CRWMS M&O (1997a, Section 4).

3.4 APPROACH AND IMPLEMENTATION OF ABSTRACTION FOR THERMAL-HYDROLOGY

This section will present the working assumptions applied to each of the process-level models used in the TH component of TSPA-VA. It provides the details of conceptual flow models for heat and mass transfer, the application of lateral boundary conditions in mountain-scale TH models, and the implementation of climate change effects. Finally, a comparison is made of select TSPA property sets to the results of the single-heater test using different conceptual flow models.

3.4.1 Development of Working Assumptions

The major working assumptions used in the TH modeling analyses are listed with reference to the section(s) in which they were applied. Additional assumptions used in the TH analyses will also be given in the text throughout the development of each individual topic. The assumptions are clearly stated during the development of each topic with reference made to the major list developed below as needed. The major assumptions detailed in this section concern the application of conceptual heat and fluid flow models, implementation of climate change, characterization of heat and mass transfer in an open emplacement drift, boundary conditions, coupled processes, and other repository design assumptions that occurred in both drift-and mountain-scale models making up the TH analyses.

The conceptual models governing heat and fluid flow are a key aspect of the model analyses and sensitivity studies. The amount and form of fracture flow, in particular, are very uncertain, and very important to most of the results. As noted by Baca and Brient (1996), it is important to use a model that allows for appropriate amounts of fracture flow. However, the choice of conceptual flow model is severely limited by computational-efficiency issues. The DKM has been selected as the preferred conceptualization of flow for TSPA-VA (see Section 2.4.3.3 in Chapter 2 of the TSPA-VA Technical Basis Document on UZ Flow), but with current computational capabilities, the DKM is practical only for one-dimensional or two-dimensional models when solving simultaneously conservation of mass and energy, and even two-dimensional can be problematical. As will be discussed, one-dimensional and two-dimensional TH simulations can be acceptable at the mountain scale, but three-dimensional simulations are necessary to obtain the waste-package variability in drift-scale results. A number of TH process-level models, and modeling approaches, have been employed to address each of the issues that were described in Section 3.2 and 3.3. As described in Section 3.1, this requires process-level models at many different scales and dimensions.

Thermal-hydrologic processes described in Section 3.2 and further elaborated on in Section 3.5.1 are addressed with the TH multiscale modeling and abstraction process which uses submodels of different dimension and different flow conceptualizations (see Section 3.5.1). The net result of the TH multiscale modeling and abstraction process is a discrete-heat source, mountain-scale, TH model (DMTH). It is an *abstracted* result that accounts for waste package variability, fracture flow in a DKM conceptualization, and edge effects of a finite-sized repository. In an approximate (or abstracted way), the DMTH result is equivalent to having discrete heat sources in emplacement drifts (for example, a drift-scale model) embedded directly in a repository-scale model that includes edge cooling processes and most large-scale heat-flow processes. With an abstracted model of this type, one can compute performance attributes of the engineered barrier system, such as waste-package temperature, waste-package relative humidity, and invert liquid saturation at many different locations in the repository. It naturally captures edge effects, responses driven by infiltration rates, and differences resulting from varying repository location within the host units. It can be used to evaluate different repository designs, including options such as backfill. This abstraction process requires four different process-level models, which will be described below. Each of the assumptions applied to the submodels making up this abstraction method is described. In its current formulation, the TH multiscale modeling and abstraction method is unable to account for large-scale heat transfer processes occurring in the gas phase and liquid phases.

Large-scale gas-phase flow processes are determined using a different TH modeling approach. Determination of gas-phase flow and air mass quantities requires a mountain-scale model including the influence of hydrology and two-phase flow processes directly. The assumptions associated with models of this type are described below. Consider first the conceptualizations required by TH models of both scales (drift and mountain).

A limited number of drift-scale TH models used the G-ECM conceptualization that allows fracture-like flow at matrix saturations somewhat less than unity. A description of how this fracture flow occurs in this conceptualized flow model is given in detail in Section 3.4.2. Most used a single vertical-fracture plane incorporated into a DKM representation of fracture-matrix interaction. The drift-scale TH models that used the DKM conceptualization were employed to generate all base-case results as well as select sensitivity studies such as a backfill repository design option. Drift-scale models making use of the G-ECM were used in select sensitivity studies only. Mountain-scale TH models were primarily two dimensional. The two-dimensional models using the generalized version of the equivalent-continuum conceptualization allow for fracture flow at matrix saturations less than unity. The two-dimensional mountain-scale models were used to develop base-case results as well as sensitivity studies.

Conceptual Flow Model Assumptions:

- The conceptual flow model applied in the two-dimensional, LDTH submodel used in the TH multiscale modeling and abstraction method is a single vertical-fracture plane DKM. This conceptual-flow assumption governs heat and mass transfer in unsaturated fractured and porous rock and is described in Section 3.4.2.3 The TH analyses based on this assumption are found in Sections 3.5.1.4 and 3.5.4.2. This drift-scale submodel results in a perimeter-averaged drift-wall temperature and relative humidity. The LDTH submodel is a component in the TH multiscale modeling and abstraction method used to develop the base-case results employed in TSPA-VA.

- The conceptual flow assumption incorporated in the two-dimensional, mountain-scale TH model used to determine repository-scale gas-phase flow and air mass-fraction data is a G-ECM. This conceptual flow assumption governs heat and mass transfer in unsaturated fractured and porous rock and is described in Section 3.4.2.2. The TH analyses based on this assumption are found in Section 3.5.4.1. The mountain-scale TH model is used to develop the base-case results employed in TSPA-VA.

- As in UZ flow (see Sections 2.4.3 and 2.4.4 in Chapter 2 of the TSPA-VA Technical Basis Document), with the exception of drift-scale models used specifically to determine water seepage into drifts, small-scale and lateral heterogeneity is not included in the TH calculations completed for TSPA-VA. Heterogeneity is thought to be essential for modeling seepage, but less important for other TH processes. Comparison of heterogeneous and nonheterogeneous calculations can provide information as to the importance of small-scale and lateral heterogeneity on TH. This topic requires further study.

- The conceptual flow model applied in a three-dimensional, drift-scale TH model used to test the TH multiscale modeling and abstraction method is a G-ECM. This

conceptual-flow assumption governs heat and mass transfer in unsaturated fractured and porous rock and is described in Section 3.4.2.2. The TH analyses based on this assumption are found in Section 3.6.1. This three-dimensional drift-scale model was developed by PA in order to test the abstraction method used to develop base-case TH results. This model is also used in a limited number of sensitivity studies.

Drift-scale modeling includes more processes than those occurring at the drift scale. The drift-scale processes must be coupled to mountain-scale processes in order to properly show, for example, that waste packages near the edge of the repository cool off faster than waste packages near the repository center. A TH multiscale modeling and abstraction method was developed to couple drift-scale processes to mountain-scale processes (see Figure 3-10). This method uses a series of four mountain-scale and drift-scale submodels to abstract the thermodynamic environment within the repository drifts at a variety of different repository locations. Additional submodels used in the approach are described below:

- The three-dimensional, SMT submodel applied in the TH multiscale modeling and abstraction method can represent edge cooling effects associated with a finite areal extent repository by means of conduction heat transfer only. It is assumed that gas-phase transfer of energy from the repository is negligible. It also assumes that horizontal and vertical condensate flow in the UZ does not significantly influence the mountain-scale temperature distribution at the repository horizon. This submodel is described in detail in Section 3.5.1.4.1. The SMT submodel provides an estimate of the average repository host rock temperature. The SMT submodel is a component in the abstraction method used to develop the base-case results employed in TSPA-VA.

- The one-dimensional, SDT submodel applied in the TH multiscale modeling and abstraction method can provide a functional relationship between the temperature of repository host rock predicted with the SDT submodel and the perimeter-averaged, drift-wall temperature predicted by the LDTH submodel. The SDT submodel is described in detail in Section 3.5.1.4.2. It is a component in the abstraction method used to develop the base-case results employed in TSPA-VA. Application of the average repository host rock temperature (SMT) in the functional relationship obtained using the SDT and the LDTH submodels results in an abstracted, line-averaged-heat-source, mountain-scale, TH model (LMTH). The LMTH model is equivalent to an abstracted model that determines average drift-wall conditions for different repository locations, including the hydrology of the system.

- The three-dimensional, DDT model applied in the TH multiscale modeling and abstraction method can represent the variability from package to package for a number of different infiltration rates and climate states using a conduction-only model. It is assumed the difference in drift-length averaged and local drift-wall temperatures is accounted for using a conduction-only heat-flow model. It is also assumed that the differences in drift-length averaged and waste-package temperatures is accounted for using a conduction-only heat flow model. The DDT submodel is described in detail in Section 3.5.1.4.4. It is a component in the abstraction method used to develop the base-case results employed in TSPA-VA. The DDT submodel provides the waste-

package-location-specific temperature deviations ΔT_{dw} from the average drift-wall temperature along the drift. Additionally, it provides the waste-package-location-specific temperature difference ΔT_{wp} between the waste package and the average drift-wall temperature along the drift.

- The perched-water zone below the repository horizon and above the water table did not greatly impact the results of TH and are hence neglected. Since the perched water serves mainly to divert flow laterally to the east, this is an important aspect for UZ flow and transport of radionuclides. In these components of TSPA-VA it is included. Since the thermal perturbation to the UZ flow field is generally short lived, it is not included in radionuclide transport through the UZ. Based on this, the perched water does not directly impact the results of the thermal perturbation. Additionally, the influence of thermal-hydrologic-chemical processes on perching is not included since this coupled process is neglected. It is possible that mineral precipitation in the fracture and matrix system can cause reduction in the overall permeability locally such that the flux of water is greater than the flow capacity of the altered region. This is a topic for future consideration in the abstraction and testing analyses for the license application. The SMT model inherently neglects the perched-water zone since it is a conduction-only model. The two-dimensional mountain-scale TH model did not include the perched-water zone since the east-west cross-section through the approximate center of the repository did not intercept the perched-water regions.

A simplified diagram describing the process-level models and the abstracted models of the TH multiscale modeling and abstraction method is shown in Figure 3-10.

The implementation of climate change is restricted to the "dry" or current climate states and the long-term-average (LTA) climate state that may result within the first ten thousand years after waste emplacement. The super-pluvial conditions considered in the UZ-flow models are not included in the TH models since this climate state scenario occurs after 100,000+ years, which is well after the repository heating effects have generally subsided. The implementation of climate change in the TH model results in new infiltration rate boundary conditions at the ground surface. The ground surface infiltration rate is a boundary condition for each of the TH models, including the hydrology component. It is not directly included in the conduction-only models. The applicable assumption for implementation of climate change in the TH models was the following:

- Climate State Assumption

  - Climate change is implemented by jumping from one set of solutions to another in a simple linear "transition" from a "dry" climate state (present-day conditions) solution to the LTA climate state solution. The results of a "dry" climate state, at postemplacement times greater than or equal to zero, represented a potential solution; and the results of a LTA climate state, at times greater than or equal to zero, represented a different solution. Transition from one solution to another occurs uniformly at times determined by the TSPA modelers. The description and implementation of this assumption is given in Section 3.4.4.

Repository design assumptions govern emplacement of different waste packages with different fuel contents and heat outputs. This includes specifications for commercial and additional wastes. The inventory and heat outputs of the DOE SNF waste packages (direct-disposal, and codisposal) are particularly uncertain. Assumptions are required regarding the heat output of the direct-disposal (or separate-disposal) waste packages and the codisposal waste packages also containing the defense HLW glass waste.

- Repository Design Assumptions

  - The heat output resulting from the DOE SNF waste is represented by the major constituent of this additional waste classification. The N-Reactor fuel represents nearly 90% of the total 2,333 MTU of emplaced DOE SNF waste. Therefore, the heat output associated with the direct-disposal waste package(s) is attributed to the N-reactor fuel decay heat. There are a total of 883 separate disposal waste packages (CRWMS M&O 1997e, p. 3-15). Four canisters of N-Reactor fuel are placed in each of the direct-disposal waste packages allotted for this fuel type. A total of 105 direct-disposal waste packages containing this waste classification are emplaced in the repository, each with an initial heat load of approximately 0.8 kW per waste package. It is assumed that the remaining 778 direct-disposal waste packages have negligible heat outputs. The total thermal load associated with the mountain-scale models is based on a total heat output from 433 N-Reactor fuel canisters.

  - The modeled number of 44 BWR waste packages in the emplacement drift segments (e.g., the drift-scale models) slightly overestimates (by 1 percent) the actual percentage of 44 BWR waste packages in the actual repository. It is assumed that this slight overestimation approximates the heat output of the Navy spent nuclear fuel to be emplaced in the repository.

  - There are 1,663 codisposal waste packages to be placed in the potential repository (CRWMS M&O 1997e, p. 3-15). Each of the 1,663 codisposal waste packages contains five HLW glass logs and one center DOE SNF fuel canister. The amount of HLW in the repository is 4,667 MTU. It is assumed that the DOE SNF fuel canister in the codisposal waste package has negligible heat output. The modeled heat output of the HLW glass log is based on a blended average of Hanford, West Valley, and Savannah River Site glass waste available for disposal. Because approximately 65 percent of the HLW is Hanford waste, the watts-per-assembly of the "blended" HLW looks very much like the Hanford waste. There are 8,314 HLW assemblies associated with the mountain-scale repository thermal load. The HLW assemblies are emplaced without any aging. See Section 3.5.3 for initial heat loads of the additional waste packages.

  - Variability of thermal output among waste packages is included to a limited extent in some of the drift-scale calculations by including seven representative waste-package types (6 full waste packages and 2 half waste packages). In mountain-scale calculations, the thermal load is smeared over the repository

footprint area and hence has no spatial variability. Variation of thermal-output history across the repository because of sequential emplacement of waste over a period of time is not considered. That is, all of the waste is simultaneously emplaced in the repository. See Section 3.5.3 for a detailed description of the base-case repository design for TSPA-VA.

The TH model domains require assumptions associated with the boundary conditions. This includes ground surface, water table, and lateral boundary conditions. Boundary condition assumptions are necessarily employed in both model scales considered.

- Boundary Condition Assumptions

  - For the TH testing models developed by PA, it is assumed that waste packages situated near the repository "center" can be modeled with a typical periodic "unit cell" drift-scale model. It is further assumed that waste packages situated near the repository "edge" can be modeled similarly, but with scaled (i.e., lower) thermal loads, as described in Chapter 4 of CRWMS M&O (1995). The thermal load scaling factor for the edge representation is developed using a solution-matching technique that reproduces the edge results from a two-dimensional mountain-scale model with a nominal thermal load using a one-dimensional mountain-scale model with a lower thermal load. The discussion and application of this assumption is given in Section 3.6.1. The PA TH models (e.g., the three-dimensional drift-scale TH models) were developed in order to test the TH multiscale modeling and abstraction method developed for near-field abstraction purposes.

  - The lateral boundary conditions associated with the two-dimensional mountain-scale models do not span the bounding fault zones (e.g., Solitario Canyon Fault to the west, Ghost Dance Fault to the east). This assumption is tested, with the results given in Section 3.4.3.

  - The two-dimensional mountain-scale, TH models and the three-dimensional drift-scale TH testing models specify the water table as a constant property boundary. This included a fixed pressure of 0.91×10^5 Pa, a temperature of 32°C, and a liquid saturation of 99.9%. The ground surface boundary conditions include a fixed pressure based on pneumo-static conditions, a temperature of 19°C, and an air mass fraction based on the fixed temperature and pressure and a relative humidity of 100%. Since the infiltration rates applied in the TH models are "net" rates already accounting for run-off and evapotranspiration, the relative humidity is set as 100% since diffusional processes to the atmosphere are already included. The infiltration-rate boundary conditions were specified as either "dry" or "LTA," climate states discussed in Section 2.4.1.1 in Chapter 2 (TSPA-VA Technical Basis Document). The climate states are identical to those applied in the site-scale models developed for UZ flow. The UZ flow model also considers a late time climate state (superpluvial) that does not influence TH due to the timing of its onset. Two-dimensional, mountain-scale, TH simulations were performed in order to investigate the TH response to an increase in water table height of

approximately 80 meters for the LTA case (see Section 2.4.1.1 Chapter 2 of the TSPA-VA Technical Basis Document). Only minor changes in the air-mass fractions and gas-flow rates were found in response to a water table rise.

The heat and mass transfer models implemented within open or filled emplacement drifts have typically been simplified based on computational efficiency limitations. The main mode of heat transfer in the open drift is radiation heat transfer.

This mode of heat transfer can be modeled explicitly or approximated by using an "enhanced" thermal conductance and then applying a conduction heat transport mechanism. Explicitly modeling radiation heat transfer in an open drift requires specific geometric information (for example, view factors) related to the radiating and receiving surfaces. For finely discretized three-dimensional dimensional systems, this requires computation of many radiation view factors associated with package-to-package, package-to-wall, package-to-floor, floor-to-wall, and wall-to-wall heat transfer. Each "radiation connection" results in a large number of nonneighboring volume element connections. The resulting coefficient matrix that has to be solved by the numerical model at each time step is inherently nondiagonal. This is particularly troublesome for the larger three-dimensional, TH, drift-scale models as computational times greatly increase.

In order to provide an efficient approximation to explicit radiation in an open drift, it is possible to compute a temperature-dependent thermal conductivity for the air elements in the model associated with an open drift. This allows for greatly increased heat transfer rates without the added burden of large numbers of nondiagonal connections typically associated with radiative heat transfer.

Heat and mass transfer by advection in an open drift also pose problems during runtime. It is typically assumed that advective flow axially in an open drift can be modeled with a porous media flow code (e.g., NUFT, TOUGH2, FEHM, MULTIFLO, etc.) by specifying a large bulk permeability along the length of the open drift. In previous TH studies, bulk permeabilities assigned to an open drift have typically ranged anywhere from 10^{-12} to 10^{-8} m^2. Using a solution from the laminar equations of motion for fully developed flow along the length of the emplacement drift, the bulk permeability should approximately approach:

$$K_b = \frac{R_d^2}{8} \approx 0.8m^2 \tag{3-1}$$

where R_d is the inner radius of an emplacement drift (= 2.55 m). This very large bulk permeability inside the drift will not allow for practical runtimes using existing flow codes. Therefore, assumptions related to the bulk permeability in an open drift were required in TH models. This assumption will govern the heat and mass transfer rates within the open drift along its axis.

- Heat and Mass Transfer Assumptions
  - The three-dimensional testing model used a thermal conduction equivalence to approximate the dominant mode of heat transfer (radiation) in an open

emplacement drift. The implementation of this simplifying assumption is given in Section 3.6.1 It is noted that the two-dimensional LDTH model used in the TH multiscale modeling and abstraction method accounts explicitly for radiation heat transfer in an open drift. This is the model used to generate base-case results for TSPA-VA.

- For the LDTH models explicitly including radiation heat transfer, it is assumed that the gas medium within the emplacement drift is a non-participating medium.

- The bulk permeability for gas-phase flow in an open emplacement drift is specified by a range of 7×10^{-12} to 10^{-8} m^2. It is assumed that if pressurization within the drift does not occur, which is the case for the selected range in bulk permeabilities (see Section 3.2.1.4), the total heat transfer rate from the waste package to the drift wall will accurately be approximated by the radiant mode of heat transfer only. The relative contribution from the convective component (refer to Section 3.6.1) is small. In the case of a rockfall-rubble-filled drift, the bulk permeability of the filled drift must assume the higher values in the given bulk permeability range since radiant heat transfer is replaced by more inefficient modes of heat transfer (for example, conduction through a low thermal conductivity rubble fill). The relative (to conduction) amount of heat removal from the waste package by convection is much more important in this case.

- Coupled Processes Assumption

  - Another important assumption was that THM and THC alterations of hydrologic properties (i.e., coupled THM and THC effects) can be neglected for the base case. This assumption is tested by means of sensitivity studies at the scale of mountain and drift. Detailed inclusion of these effects will be left to future work (i.e., TSPA-LA). Initial THM, THC, and rockfall sensitivity studies are included in Section 3.6.

3.4.2 Conceptual Flow Models

The unsaturated porous medium contains both fractures and rock matrix, each with its own set of characteristic properties. Typical conceptual models used to characterize such a system include an ECM (i.e., an equivalent porous medium with averaged fracture and matrix properties), a DKM (i.e., a porous medium containing separate fracture and matrix continua), and a random, discrete fracture model. The ECM and the DKM are continuum models that represent the fracture domain in an idealized manner. The ECM (and more advanced single permeability approaches such as the G-ECM) characterizes the matrix rock and fracture properties through an "effective" set of properties, while the DKM uses separate and distinct matrix and fracture domains and properties.

3.4.2.1 Equivalent Continuum Model

The ECM assumes that pressure and thermal equilibrium exist between the fractures and matrix. The fracture and matrix properties are fracture pore volume averaged to produce parameters that

represent a single effective porous material. The effective porous material can behave as matrix or fracture depending on the phase of the fluid and the bulk liquid saturation of the effective material. For properties typically associated with fracture and matrix, the fracture domain will remain at its residual saturation for almost all values of capillary pressure associated with the matrix material. Not until the matrix is almost fully saturated and the capillary pressure is reduced to near zero will the fracture saturations increase and the water in the effective material begin to flow at bulk properties similar to those of the fracture domain. This assumption inherently requires that water completely fill the pore space of the matrix before it flows "like" a fracture. Previous TH studies have indicated that condensate shedding, a result of repository heat-driven processes, can occur in regions with matrix saturations somewhat below fully saturated. This process is a nonequilibrium process; therefore, it cannot be captured when the chosen flow model requires equilibrium between fracture and matrix. The mathematical ECM formulation is given here since it also governs the application of the volume average quantities obtained with the use of the G-ECM.

Using an ECM formulation for heat and mass transfer, effective material properties can be defined as the following (Ho and Eaton 1994; Peters and Klavetter 1988):

$$\phi_b = \phi_f + (1-\phi_f)\,\phi_m \tag{3-2}$$

$$S_b = \frac{S_f\phi_f + S_m(1-\phi_f)\phi_m}{\phi_f + (1-\phi_f)\phi_m} \tag{3-3}$$

$$K_b = K_f\phi_f + K_m(1-\phi_f) \tag{3-4}$$

where ϕ_b is the effective porosity, S_b is the effective liquid saturation, K_b is the effective (bulk) permeability, all a function of the rock matrix (subscript m) and fracture (subscript f) properties.

Additionally, the equations used in the ECM to calculate the water phase relative permeability ($K_{r,w}$) and the capillary pressure (P_c) are (van Genuchten 1980):

$$K_{r,w} = (S^*)^{1/2}[1-(1-(S^*)^{1/\lambda})^{1/\lambda}]^2 \tag{3-5}$$

$$P_c = 1/\alpha[(S^*)^{-1/\lambda}-1]^{-1/\beta} \tag{3-6}$$

where S^* is the scaled saturation, α is the van Genuchten air entry scaling parameter, β is the van Genuchten pore size distribution parameter, and λ is $1-1/\beta$.

The scaled saturation is defined as:

$$S^* = (S_l-S_{lr})/(1-S_{lr}), \tag{3-7}$$

where S_l is the liquid saturation and S_{lr} is the residual water saturation. Note the application of 1.0 in the denominator of the scaled saturation definition used in the standard ECM. The effective continuum liquid phase relative permeability is:

$$K_{b,r} = \frac{K_{r,m}K_m\left(1-\phi_f\right)+K_{r,f}K_f\phi_f}{K_b} \tag{3-8}$$

where $K_{r,m}$ and $K_{r,f}$ are given by Equation (3-5) for fractures and matrix and the effective continuum gas-phase relative permeability is typically taken to be 1 -$K_{b,r}$. The standard ECM was not used in the TSPA-VA TH calculations. Each of the models used for the VA, either abstraction testing models or the TH abstraction methodology models, applied alternative conceptual models such as the G-ECM and the DKM. This was necessary in order to ensure increased fracture flow processes during the heating simulations.

3.4.2.2 Generalized-Equivalent Continuum Model

The G-ECM is a modification of the ECM formulation where the matrix is allowed to "saturate" at a value less than unity. This modification allows fracture-like flow to occur without requiring the matrix to be nearly saturated. This is accomplished by specifying the matrix satiation saturation parameter (S_{ls}) which can take on a value less than the 1.0 used in the standard ECM formulation. However, temperature and pressure equilibrium are still assumed in both of the conceptual models. This implies that in dryer than ambient regions (a result of repository heat), the flow that may have been in the fractures will be drawn back into and held by the matrix because of its strong capillary potential. However, even with this limitation, more water will return through the dryout zone (both through condensate movement and normal infiltrating water) through the fractures of these alternative conceptual models than the ECM. The G-ECM will also allow for increased fracture flow at ambient liquid saturations. This is especially useful when the infiltration rates at the ground surface are high (on the order of 1 mm/year and above) and the matrix liquid saturations are less than fully saturated. Consequently, the G-ECM assumption allows one to consider much higher infiltration rates at the ground surface than in an ECM while still maintaining an UZ in which the repository heat is emplaced.

The equations for the effective porosity, the effective liquid saturation, the effective bulk permeability, and the effective continuum liquid phase relative permeability (Equations [3-2] through [3-4]) hold in the G-ECM. The gas-phase relative permeability used in the simulations was set equal the fraction of pore space that was not occupied by water or:

$$K_{r,g} = 1\text{-}S^*_{l,f} \tag{3-9}$$

The water phase relative permeability, the capillary pressure, and the bulk permeability equations are the same as would be used in the ECM (Equations [3-5], [3-6], and [3-8]) but the scaled saturation, S^*, has been modified to allow the rocks to satiate at a value less than unity. The new scaled saturation is defined as:

$$S^* = (S_l\text{-}S_{lr})/(S_{ls}\text{-}S_{lr}) \tag{3-10}$$

where S_l is the liquid saturation, S_{lr} is the residual water saturation, and S_{ls} is the satiation saturation.

All of the rock properties used in the G-ECM TH simulations were taken from 14 rock property sets created by inversions (preliminary base-case property set can be found in DTN

LB971100001254.002, DTNs for other property sets are located in Table 3-3) and a set of thermal properties (DTN SNT05071897001.002). The fracture satiation saturations, $S_{ls,f}$, were all set to 1.0 as specified in the UZ flow task, Chapter 2 of the TSPA-VA Technical Basis Document. The matrix satiation saturation values for the two-dimensional mountain-scale simulations as well as the three-dimensional drift-scale TH simulations were generated using TOUGH2 one-dimensional DKM simulation results. The one-dimensional DKM column was extracted from the two-dimensional mountain-scale cross section at the location northing = 233,400m and easting = 170,525m. This corresponds to the location on the northing = 233,400m cross section that had the highest base-case infiltration rate of 18.9 mm/year (DTN GS960908312211.003, this datum is qualified). The one-dimensional DKM model was then run to steady state (10^6 years), and the average liquid saturation value for matrix elements in each geologic unit was calculated. In the G-ECM, the matrix satiation saturations were all set to 1.0 in the nonwelded units (Paintbrush Tuff, Calico Hills, Bull Frog-vitric 3, Tram Member-vitric 3, Prow Pass-zeolitic 2, and Bull Frog-zeolitic 2). In the welded units (Tiva Canyon, Topopah Spring, and Prow Pass-vitric 3), the satiation saturation was set equal to (1+average matrix saturation)/2. This process was repeated for each of the property sets using the present day climate infiltration values. The satiation saturations for the three preliminary base-case property sets are plotted in Figure 3-11. The same satiation saturations sets were also used for the higher infiltration climate change simulations.

The G-ECM was used in both the two-dimensional mountain-scale simulations that yielded air mass fractions and gas-flow rates and the three-dimensional drift-scale simulations that were used to test the results from the TH multiscale modeling and abstraction method.

3.4.2.2.1 Optimal Satiated Saturation Value

The satiated matrix saturation is a threshold saturation beyond which the matrix cannot accept any more water. Thus, the upper bound matrix satiation saturation, which is the ECM limit, is unity. A matrix satiation saturation of unity is used in the nonwelded units because of their high matrix permeability and general sparseness of fracturing. On the other hand, the matrix can be considered to be currently at or below the satiated saturation level for the welded units. The lower bound for S_{ls} can thus be taken to be the average matrix saturation from measured borehole data.

RamaRao et al. (1998) found good agreement among measured borehole data, DKM results, and G-ECM predictions using a satiated saturation value defined by the average of these two bounds or S_{ls}=0.5(1+ average matrix saturation). This showed good agreement between the matrix liquid saturation vs. depth and the borehole data for the G-ECM model predictions using the adjusted values of the satiated saturation and the "calibrated" DKM model results based on the parameters given in Bodvarsson et al. (1991, pp. 6-12 to 6-14, p. 6-26, pp. 7-8 to 7-9).

Recall that the adjustable parameters in both the DKM and the G-ECM formulations are related to the strength of the fracture-matrix interaction. In the DKM approach (described in Section 3.4.2.3), this is achieved by specifying a reduction factor $f(S_{up})$ for the geometric fracture-matrix connection area. In the G-ECM approach, the same effect is obtained by setting a matrix satiation value (S_{ls}). A layer-by-layer comparison of these two quantities indicated that

the two adjustable parameters $f(S_{up})$ and S_{ls} are indeed consistent, and can generally be correlated to the degree of welding in the layer of interest.

3.4.2.3 Dual Permeability Model

The DKM is a conceptual flow model that allows for nonequilibrium fracture-matrix flow processes. This is the primary advantage of the DKM over the ECM and G-ECM. It introduces separate fracture and matrix domains each, with its own set of hydrologic properties. Capillary-pressure equilibrium is not required so fracture saturations are not restricted by the value of capillary pressure in the matrix domain. Therefore, liquid flow in the separate fracture domain is not subject to a specific matrix saturation as is the case for the ECM and G-ECM. In the DKM, heat, gas, and liquid are allowed to flow between the fractures and matrix, as well as through each continuum separately. The DKM is generally more applicable to a wider range of flow problems (e.g., transient flows, high infiltration rate boundaries); however, the DKM requires additional information related to the coupling between the fracture and matrix continua (Ho 1997). An added complexity is that the coupling between fracture and matrix must account for both heat and mass flows, not just mass flow as in typical ambient flow problems.

The flow (gas, heat, and liquid) between fractures and matrix, in general, can be written as the following:

$$Flow = (\text{property conductance})x(\text{geometric conductance})x(\text{driving potential}) \tag{3-11}$$

where the geometric conductance term is modified in DKM to account for heterogeneities, flow fingering, and preferential wetting between fracture and matrix in the case of liquid and gas-phase flows. Heat flow should maintain a full geometric conductance area, A, although previous studies indicate that heat flow is not very sensitive to the reduction (coupling) factor applied to the liquid and gas-phase flow geometric conductances (Ho 1997). The geometric conductance may take the following form:

$$\text{geometric conductance} = \frac{\mathrm{A}}{\mathrm{d}} f\left(S_{up}\right) \tag{3-12}$$

where A is the area available for liquid, gas, and heat flow; d is the nodal distance between fracture and matrix elements; S_{up} is the saturation in the upstream element; and $f(S_{up})$ is the term that indicates the amount of coupling between fractures and matrix. The coupling factor typically takes the form (Ho 1997):

$$f\left(S_{up}\right) = \begin{cases} C \\ S_{up}^{n} \\ k_r\left(S_{up}\right) \end{cases} \tag{3-13}$$

The first form of the fracture-matrix multiplier, $f(S_{up})$, is a constant, C, independent of liquid saturation. The second factor is an upstream saturation raised to the power n. The final factor is

the upstream relative permeability. Additional details related to the results and testing of this conceptual model can be found in Section 2.4.3.3 in Chapter 2 of the TSPA-VA Technical Basis Document. For TH base-case calculations performed using the TH multiscale modeling and abstraction method, a constant factor specified in Equation (3-13) was selected based on inversion results.

The DKM applied in the two-dimensional LDTH model used in the TH multiscale modeling and abstraction method was in the form of a single vertical fracture plane adjacent to a separate matrix domain. The model domain in the (X-Z) plane (cross section) contains details of the waste package, drift wall, drift-to-drift spacing, and the layering from the ground surface to the water table. The third dimension (Y) provides a means for an implementation of the DKM in the NUFT code (Nitao 1996). The fracture domain is 1×10^{-3} m wide, with the adjacent matrix domain 1 m wide. The surface infiltration rate is input into the fracture elements located at the ground surface of the model. Fracture-fracture, matrix-matrix, and fracture-matrix flows are all possible in the LDTH model. This includes both mass and heat.

3.4.3 Evaluation of the Lateral Boundary Conditions in the Two-Dimensional Mountain-Scale Models

Two-dimensional TOUGH2 G-ECM simulations were performed to determine the air mass fractions and the gas-flow rates near the repository. The simulation domain of the two-dimensional cross section consisted of 2,816 active elements and extended from easting = 169,937.5 m to 171,362.5 m at northing = 233,400 m. The domain extended to, but did not include, either the Solitario Canyon fault to the west or the Ghost Dance fault to the east. The boundary conditions for the eastern and western boundaries of the simulation domain did not allow mass or heat fluxes. To verify that the exclusion of the fault zones and the no-flux boundary conditions did not affect the simulation results near the repository, a larger simulation domain that included the two faults was prepared and a simulation was run using the preliminary base case (DTN LB971100001254.002) property set. This data set is qualified.

To model the faults, a column of elements was added on both the western and eastern edges of the two-dimensional cross section. Each column of elements was 25 m across. The fault zones were created by duplicating the western edge column centered at easting = 169,950 m at easting = 169,925 m and by duplicating the eastern edge column centered at easting = 171,350 m at easting = 171,375 m. The infiltration rates over the faults were set to be the same as that over the adjacent column. The fracture permeability of the fault elements was increased by two orders of magnitude, and the matrix permeabilities were kept constant. The offset of the stratigraphic layers because of fault movement was not included in the simulation.

The air mass fraction and temperature have been plotted as a function of time for elements at the center (easting = 170,650m) and at the eastern edge of the repository (easting = 171,200 m). Figure 3-12 and Figure 3-13 show the air mass fraction history for the elements at the center and the eastern edge of the repository for the cases run with and without the bounding fault zones. There are very minor differences in time or magnitude between the air mass faction profiles.

Figures 3-14 and 3-15 contain the temperature histories for the center and the eastern edge repository elements for both the case with and without the bounding fault zones. Again, there are only minor differences between the center and edge elements in the two simulations.

Figures 3-16 through 3-19 present gas fluxes across the simulation domains at 100 and 1,000 years for the simulation domains with and without bounding fault zones. The scale of the length of the gas-flux vectors in all four plots is identical. The highest gas-flux vectors at 100 years are 2.46×10^{-6} kg/m^{2}s for the simulation domain without faults and 2.44×10^{-6} kg/m^{2}s for the case with faults. A comparison of the gas flow fields shows that the addition of the vertical faults on both sides of the simulation domain does not introduce large-scale circulation into the simulations. At 1,000 years, the greatest gas fluxes are 5.25×10^{-7} kg/m^{2}s for the simulation domain without faults and 5.35×10^{-7} kg/m^{2}s for the case with faults. Again, the presence of the faults has not appreciably changed the gas-flow field around the repository. Combined with the air-mass fraction simulation results presented in Figures 3-12 and 3-13, the absence of the faults in the simulation domain has not affected the information that is being abstracted from the two-dimensional mountain-scale G-ECM simulations.

3.4.4 Implementation of Climate Change in the Thermal-Hydrological Analyses

The "dry" or present day climate state is compared to the LTA or "wet" climate state in a transient boundary condition analysis. The initiation of the LTA climate state is thought to occur within the first 10,000 years after the emplacement of repository wastes. In order to establish the manner in which waste-package-specific variables (e.g., temperature, relative humidity) transition from the "dry" climate solutions to the "wet" (LTA) climate solutions, the three-dimensional, testing drift-scale TH model uses *transient* ground surface infiltration boundary conditions initiated at several times after waste emplacement. The results of this study (using the testing models) are used only to determine the appropriateness of the climate state transitioning method specified in the base-case computational procedure applied in the TH multiscale modeling and abstraction method. This method involved computing waste package and emplacement drift response curves separately for present day climate and LTA climate states and treating climate state transitions as a uniform jump from the present day climate solution to the LTA climate solution.

The plan view location of the testing model domain was northing coordinate = 233,400 m, easting coordinate = 170,650 m. Four cases were considered: transition to LTA climate at 100 years, 500 years, 1,000 years, and 10,000 years after waste emplacement. A final baseline case allowed for the onset of the LTA climate state at the time of repository closure (t = 0 years).

Temperature comparisons for the climate change study are made at the surfaces of the design basis 21 PWR (the hottest waste package in the TH models), the cold 21 PWR, and the direct-disposal waste package containing four canisters of separate disposal DOE SNF (the coldest waste package in the TH models). A relative humidity comparison is performed for the cold 21 PWR waste package. Table 3-6 details the infiltration rate boundary conditions applied to the three-dimensional drift-scale model used in the transient climate change analysis.

As an example of a transient climate change boundary condition, consider a transient climate change from "dry" to LTA at 500 years after waste emplacement:

$$q = 11.5\frac{mm}{yr}; 0 \le t \le 500\,yr$$
$$q = 59.2\ \frac{mm}{yr}; 500 < t \le 100{,}000\,yr \qquad (3\text{-}14)$$

Referring to Figures 3-20 through 3-23, note that transition from the "dry" solution to the "wet" solution occurs in a relatively smooth manner. For the nominal infiltration rate and climate change state, the transition occurs gradually in approximately 100 years or less. For higher infiltration rates the transition is faster, for lower infiltration rates it is slower. Based on these results, it was assumed that the "dry" climate and "wet" climate solutions can proceed from an initial waste emplacement time of t = 0 years. One can move from solution-to-solution depending on the appropriate climate state specified in the total system calculations.

Climate change considerations were also included in the two-dimensional mountain-scale TH models used to determine the gas-phase flow rates and air mass fractions for repository center and edge. The spatial variability of the infiltration rate boundary condition shown for an east-west cross-section at a northing coordinate of 233,400 m is given in Figure 3-24 for the nominal infiltration rate and its associated climate change. The average infiltration rate for the "dry" climate model was ~ 7.96 mm/yr. The average infiltration rate for the "wet" climate model was ~ 45.3 mm/yr. Recall that these averages are specific to the east-west cross section selected for the analyses

3.4.5 TSPA Property Set Comparison to the Results of the Single-Heater Test

The measured temperature results from the Yucca Mountain Project single-heater test have been applied directly to decisions made regarding the hydrologic property sets used by TSPA. The hydrologic property sets characterize the UZ flow fields used in TSPA-VA. The resulting UZ flow fields are then applied in the UZ transport of radionuclides from the repository horizon to the SZ. Therefore, the hydrologic property sets govern the flow characteristics of fluids through the UZ and hence the movement of radionuclides to the water table. This is an important aspect of TSPA. Therefore, it is necessary to make comparisons of hydrologic property sets used in TSPA to known quantities. This serves to increase our confidence in subsequent model predictions.

The Exploratory Studies Facility single-heater test is located in the Topopah Springs Middle NonLithophysal (Tptpmn) unit. This is one of three possible repository host rock units. This experiment represents the first heater test located within an actual repository host unit. Therefore, it provides relevant data associated with heating and subsequent cooling processes occurring directly in a repository host unit. It also provides valuable information to be used in both property set verification and conceptual flow model validation. The results of the single-heater test are used directly in the TSPA analyses.

TSPA-VA has developed alternative property sets in order to describe the natural property uncertainty in the geologic system. Each of the property sets is developed using model inversion so that the ambient matrix saturations and matrix potential are reproduced by the properties. This is done by fixing experimentally determined matrix properties (obtained from drainage

experiments) and varying fracture properties, including the interaction parameter between fracture and matrix rock. Each of the calculated property sets reproduces ambient conditions of the mountain. For completeness, some of the property sets are also tested against the single-heater test results. Two of the hydrologic property sets used in TSPA-VA, the preliminary base case and the base case, have been compared directly to known heating results of the single-heater test. It is noted that the heating processes driven by the single-heater test include both drying and rewetting. Therefore, hysteresis of the matrix and/or fracture characteristic curves governing the capillary pressure and relative permeability may be important. The rock properties applied in the TSPA-VA originated from drainage experiments only so hysteretic effects are not included in any of the calculations.

The property sets under consideration contain different fracture capillary characteristics as well as fracture and matrix rock interaction parameters. Table 3-7 indicates the matrix and fracture properties associated with the single-heater test location for both the preliminary base case as well as the base-case property sets used in TSPA-VA. The differences are highlighted. Table 3-8 provides the thermal properties applied to this location as well.

The property set comparison is performed using both ECM and DKM conceptualizations of the single-heater test. Each conceptualization uses identical property sets, so a total of four simulations are performed: two for the base case (ECM and DKM), two for the preliminary base case (ECM and DKM). Therefore, this comparison allows not only a hydrologic property set verification, but a first step for conceptual model validation for heating processes as governed by the hydrologic properties used in TSPA-VA. A description of the single-heater test model domain is given in detail in Francis et al. (1997b). Although described specifically for an ECM conceptualization, this same model domain is adapted, based on Ho (1997) for a DKM conceptualization. This comparison is made so as to ascertain the appropriateness of the TSPA-VA property sets with respect to the single-heater test results.

A general description of the single-heater test model follows. It is assumed that the surrounding single-heater test block contains homogeneous fracture and matrix rock properties. Fracture features, in particular those found near the end of the five-meter-long heater, are not included. Since the modeled block is homogeneous and symmetric through the center of the heater, only half of the single-heater test block is modeled. The heating element is located in a five-meter-long borehole approximately two meters from the front face of the thermomechanical alcove. The model faces adjacent to this alcove and the thermomechanical alcove extension are insulated boundaries. The insulation covering the exterior rock faces reduced the amount of heat flow out of the test block. It is assumed in the model analysis that the insulation is an effective vapor barrier. The thermodynamic properties (the temperature, gas-phase pressure, and air mass fraction) of the alcoves are fixed in time in the model. The model boundaries in the rock above and below the heater are located sufficiently far from the heat source that the thermal perturbation does not reach the boundaries during the duration of the simulation. The lateral boundary conditions are the equilibrated results from the ambient initialization procedure. They are also kept constant in time but vary with depth as a result of gravitational effects. A no-flux boundary condition is specified along the plane of symmetry.

For the DKM simulations, the equilibration procedure determines both fracture and matrix initial saturations at steady-state conditions. The fixed saturation boundary (fracture and matrix)

applied in the equilibration procedure of the single-heater test model is obtained from a one-dimensional mountain-scale DKM that contains the stratigraphy of the entire mountain from ground surface to water table. This model contains the same geologic layering and property sets used by TSPA. The one-dimensional ambient initialization is performed once for each property set. The one-dimensional mountain-scale model is carried out to steady state for the nominal infiltration rate to determine initial fracture and matrix liquid saturations. The resulting steady-state matrix and fracture saturations are placed in the single-heater test model and further equilibrated using TOUGH2 with the lowermost boundary in the model domain fixed. The results of a single-heater test equilibration process are steady-state temperature, liquid saturation of fracture and matrix rock, and gas-phase pressure. These are the initial conditions for the heating simulations using TOUGH2.

The heat input into the single-heater test was approximately 3.86 kW for the nine-month heating cycle. This was followed by an eight-month-long cooling period. This same heating and cooling sequence is applied to the single-heater test model simulations.

The results of TSPA property set and conceptual model comparison to the measured results of the single heater test after 275 days of heating are shown in Figures 3-25 and 3-26. The measured data in the these figures represent all thermocouple locations (over 300) used to measure temperature during the test. Therefore, represented thermocouple locations are above, below, and in a direction perpendicular to the heater axis (to the side). Radial temperature profiles and temperature-time histories from the model are compared to the measured data at different locations in the single-heater test block. The model results marked as "up" in the figure represent model results through the heater midplane in a direction vertically upward from the axis of the heater. This is in a direction opposite of gravity. Model results marked "down" represent model results at the heater midplane vertically downward from the axis of the heater. This is in the same direction as gravity. Model results marked "sideways" represent model results in the horizontal direction towards the thermomechanical alcove extension in the direction of the insulated surface. It is at a right angle to the gravity vector in a direction perpendicular to the heater axis. Time history data are compared at heater midplane.

The preliminary base case and the base-case hydrologic property sets (applied in both ECM and DKM) allow for anisotropic fracture permeability fields (see Table 3-7). The vertical bulk permeability for both property sets is $\sim 7 \times 10^{-12}$ m^2, and the horizontal is $\sim 4 \times 10^{-13}$ m^2, which is over a full order of magnitude greater in the vertical direction.

Asymmetrical heating occurs as a result of preferential gas flow resulting from the anisotropic permeability fields. Since the resistance to flow is lower in the vertical direction, heated gas is more likely to flow vertically rather than horizontally. The energy flow in the horizontal direction (sideways) is dominated by diffusion (e.g., conduction heat transfer and energy transfer by mass diffusion as evidenced by the shape of the temperature profile shown in Figure 3-25 and Figure 3-26). Gas-phase pressure gradients push water vapor from the heat source radially away in all directions. Density differences between steam and air will force the steam around the heater element to rise. Consequently, the rate at which steam moves vertically away from the heater will be determined by both the outward pressurization resulting from vaporization of water and the upward forces resulting from gas-phase density gradients developed upon heating.

In the sub-boiling regions above the heater, gas-phase convection transports energy upward from below the heater by natural (buoyant) convection. That is, the model develops a natural convection flow pattern in which heated gas from below rises vertically upwards (through the fractures) taking its heat along with it. Vertical flow can proceed past the heater through the dryout zone into the sub-boiling region above since there is no longer a source of water to vaporize locally (for ECM or DKM). It can transition through condensation that may be present since the gas-phase relative permeability is nonzero there.

The temperature in the dryout zone above the heater is slightly lower than the temperature in the dryout zone directly below the heater. This is a result of an additional energy requirement needed to drive the more extensive heat pipe above the heater than below. The heat-pipe zone above the heater is larger because it uses gravity to sustain its development (i.e., liquid flow back to the heat source from above by capillarity and gravity). Below the heater, the refluxing is driven by capillary forces alone; gravity does not drive water back to the dryout zone. The refluxing process is a constant temperature process characterized by liquid- and vapor-phase counterflow. Liquid flows towards the dryout zone where the capillary suction is the highest; vapor flows away from the dryout zone by pressure gradient radially outward and by density gradient above the heat source. This counterflow process proceeds with a continual source of water (liquid return at dryout and vapor return at condensation). It is in the previous discussion (and the extent to which these processes proceed) in which the ECM and the DKM results tend to diverge.

The ECM tends to "lock" water into the system by requiring a fully saturated matrix before the fractures are allowed to efficiently flow and drain water out of the system. Water vapor (driven by pressure gradients and density variations in a gravity field) is moved from the drying zone where it condenses both above and below the heater just outside of the boiling front surrounding the heater. The matrix then imbibes the water before it can drain through the fractures. Capillary forces and gravity (above the heater) then draw water back to the dryout zone where vaporization occurs. Capillary forces alone drive this process below the heater. This process will occur at a the boiling temperature of water at the total pressure of the system (96°C at the repository). This process is called refluxing. (Refluxing is thought to be a characteristic of the ECM model and has not been found experimentally).

This water "locking" phenomenon is greatly diminished in the DKM model. Only slight refluxing occurs (and mainly above the heater) as the water that condenses from the vapor phase enters the fracture continuum and drains from the system.

The temperature profile in the DKM simulation does not flatten as much at the boiling point as does the ECM simulation (see Figure 3-27). The temperature smoothly progresses through boiling for each of the DKM cases considered. This is a result of two mechanisms. First, very little refluxing is predicted. Water that enters the fractures can flow out of the system. The second mechanism is the pressurization of the matrix elements. Since the matrix permeabilities are a very low 4×10^{-18} m^2, vaporized matrix water is not able to advect to the fractures . This is thought to result in a buildup of pressure in the matrix elements. Higher pressures in the matrix are thought to allow water to exist in a liquid form at temperatures higher than can exist at ambient conditions.

Reference to the time-history plots, as shown in Figures 3-27 through 3-29, compare ECM to DKM using two TSPA property sets. Note that the DKM temperature predictions at the thermocouple (a temperature measuring device used in the single-heater test) nearest the heater increase initially very rapidly with a much slower rate of increase with continued heating. ECM temperature predictions at this location increase slowly initially and with a faster rate of increase at later times.

Initially, the DKM proceeds through the boiling point (much like the data) without flattening at 96°C as predicted by the ECM cases. As refluxing occurs in the ECM models, the predicted temperature 0.41 m to the side of the heater is suppressed as energy taken from a small dryout zone is required to run the refluxing process going on above/below it (refer to Figure 3-29). The constant temperature refluxing zone is located directly above/below this location (see Figure 3-27 and Figure 3-28). The temperature in the DKM is not suppressed because the matrix can pressurize, allowing higher equilibrium temperatures before dryout occurs. It is noted that the energy requirement to run the refluxing zone (like in an ECM) is greater than the cooling associated with water passing back through the fractures near the dryout zone (like in a DKM). Hence, temperatures predicted by the DKM are greater than the ECM during the first 100 days of heating at this location very near the heater.

As heating proceeds, the boiling front moves away from this location and, in effect, the refluxing process moves away from the heater (in the ECM). The energy requirement near the heat source is reduced as the refluxing zone moves further away and the dryout zone continues to grow. Consequently, the temperature predicted by the ECM at 0.41 meters from the heater begins to rise at a faster rate than that of the DKM (at late heating times). In the ECM, liquid water cannot return to the dryout zone until the temperature returns to the two-phase equilibrium temperature. In the DKM, steam that moves from the matrix to the fractures is transported away from the dryout zone where it can condense and possibly drain from the system. If the fractures do not pressurize, liquid water cannot exist if the temperature exceeds the nominal boiling point. Conversely, water and its vapor can exist in the pressurized matrix rock long after the fractures have dried out. Once matrix dryout has occurred, the thermal conductivity of the matrix will decrease because the thermal conductivity of water is higher than that of air or steam. A result of this is that at late heating times, the ECM predicts higher temperatures than the DKM at locations near the heat source because the rate of conduction heat transfer away from the dryout zone 0.41 m from the heat source is lower in the ECM than in the DKM.

The temperature predictions at thermocouple locations even further from the heat source (see Figure 3-28) further illustrate this result of the ECM. It takes 125 days or longer for the dryout zone to reach 0.7 m below (or above) the heater. This is consistent with a reduced rate of heat transfer from the dryout zone near the heater as well as the energy requirement needed for phase change. The slow dryout front movement results in lower temperatures for the entire nine-month heating cycle. The DKM predicts higher temperatures and heating at a faster rate at thermocouple locations farther away from the heater. This more closely approximates the actual heating trends of the measured data. In the ECM, refluxing at the outer locations is removing energy from the system at such a rate that the rate of temperature increase is retarded as evidenced by the constant temperature regions occurring at the fringe of the dryout zone during refluxing. This large reflux region is not seen in the measured data. Therefore, based on the above analysis, the DKM conceptualization of heat and mass flow is recommended.

As indicated above, the dual permeability conceptualization more closely approximates the results of the single-heater test. Additionally, it is noted from the same figures that the TSPA-VA base case hydrologic property set, when used in a DKM formulation, more closely approximates the heating results of the single-heater test. Therefore, the base-case thermal and hydrologic property set better (than the preliminary base case) reproduces both ambient conditions of the mountain and the heating and cooling processes initiated during the single-heater test. The resulting comparison to the single-heater test data guided, to a certain extent, the decision to move from the preliminary base-case property set to the base-case property set applied in calculations supporting TSPA-VA.

Some additional comments remain. It is noted from the comparison that, although the heating trends of the DKM more accurately represent the heating trends of the measured data than do the results of the ECM, the DKM still tends to underpredict the temperature measurements taken at specific locations from the single-heater test. Two possible reasons are postulated to explain the discrepancies; fracture spacing and vapor pressure lowering. Fracture spacing is a direct input in the DKM conceptualization and is a measure of the distance between fractures. It is a measure of the flow resistance of vapor transfer as it leaves the matrix block and enters the fracture element. For pore water located in the matrix, heating occurs in the matrix and subsequent evaporation transfers the water vapor from the matrix to the fracture. The fracture-matrix flow rate for the gas phase varies as the following:

$$F_g \propto \frac{k_m A_g}{d} \tag{3-15}$$

where k_m is the intrinsic matrix permeability, A_g is the conductance area for gas, and d is the nodal distance between fracture and matrix rock. The driving force is the gas-phase pressure difference. The conductance area for the gas phase goes essentially unmodified. It is almost a full geometric conductance because the fracture liquid saturation is typically low. The interaction parameter between fracture and matrix rock is applied to the liquid flow only. The nodal distance, d, is proportional to the fracture spacing. The fracture spacings applied to the TSPA property sets and used to estimate ambient flow (see Table 3-7) are also used in the DKM simulations of the single-heater test. The fracture spacings are applied to model inversions (see Section 2.4.3.1.2 in Chapter 2 of the TSPA-VA Technical Basis Document) at the scale of the mountain and were used to reproduce information such as ambient borehole matrix saturations. Therefore, they are used to characterize the attributes of ambient flow on a much larger scale. The single-heater test occurs on a much smaller scale. It is conceivable that the size or frequency distribution of participating fractures at the scale of the single-heater test was not the same as that at the scale of the mountain. If the effective fracture spacing was to increase, then the flow area per unit volume for the water vapor to flow from the matrix to the fracture would be reduced. This would cause a larger pressurization of the matrix block, resulting in even higher temperatures. Therefore, increasing the fracture spacing would increase the temperatures around the heat source and could bring them more in line with the measured values.

Alternatively, if the fracture spacing decreased, dryout would occur more readily near the heat source, resulting in a lower dry thermal conductivity. This reduces the heat transfer rate by conduction from the dryout zone and increases the temperature there. Because refluxing is

minimal in the DKM, energy leaving the dryout zone (although now at a lower rate) will not be used in a two-phase counter flow process so that temperatures increase without flattening at the nominal boiling point. That is, pressurization still occurs because the conductance between fracture and matrix rock is still finite (unlike in an ECM). These descriptions describe similar results by contrasting means. At this time, it is unclear by which means the modeled results would more accurately represent the measured data or which description is the driving mechanism during drying. One way to determine the correct (or driving) mechanism is to determine the drying characteristics of the matrix pores based on a measured liquid saturation. Does the matrix pore space contain water above the nominal boiling point? If the matrix rock contains liquid water at high temperatures, this indicates rock pressurization, which lends evidence to widely spaced participating fractures in the single heater test. If the matrix rock is essentially dry at the nominal boiling point, this may lend evidence to more closely spaced participating fractures and lower heat transfer rates from the dryout zone (and not as much pressurization).

Vapor pressure lowering associated with increasing capillary pressures can result in a difference between simulation results and experimental data. In the analysis described above, lowering vapor pressure will change the two-phase water/gas equilibrium temperature in the matrix elements. Surface tension effects will cause the wetting fluid in the matrix to be at a lower pressure than the non-wetting fluid. The difference in pressures will depend upon the surface tension of the fluid, the radius of curvature of the liquid/vapor interface, and other phenomenon. The effect of vapor pressure lowering on fluids in a porous media is that, at a given temperature, the equilibrium vapor pressure is less than would be the case when the vapor and liquid pressures are the same. As an example, liquid water will boil at 100°C at one atmosphere pressure. If the water is allowed to imbibe into a porous medium, the water would, depending on the saturation and permeability of the porous medium, boil in situ at a temperature greater than 100°C at one atmosphere. Consequently, including lowering vapor pressure effects in the ECM and DKM simulations might yield the higher temperatures that were seen in the single-heater tests.

3.5 THERMAL HYDROLOGY BASE CASE FOR TSPA-VA

3.5.1 Description of Models and Processes Used in the Thermal-Hydrologic Multiscale Modeling and Abstraction Method

3.5.1.1 Background

The TH multiscale modeling abstraction method is used to develop time-varying estimates of key NFE performance measures for locations throughout the repository. Performance predictions vary significantly for different locations because of differences in hydrostratigraphy and infiltration flux. The performance measures include drift-wall temperature, waste-package temperature, and drift-air relative humidity at the waste-package surface (see Table 3-9). The estimation procedure is fast enough to be conducted for many locations in the repository layout and repeated for TSPA-VA sensitivity cases and alternative model exercises.

Measures calculated for TSPA-VA are indicated in Table 3-9 by bold, uppercase X. Other measures also calculated by the approach are indicated by lowercase x. The measures are temperature (T), relative humidity (RH), gas-phase air mass fraction ($X_{air,gas}$), liquid-phase

saturation (S_{liq}), and liquid-phase flux (q_{liq}). Although the TH multiscale modeling and abstraction method produces air mass fraction information, TSPA-VA abstracts all gas-phase data (for example, air mass fraction, vertical and horizontal gas-phase mass flux) from the two-dimensional mountain-scale TH models described in Section 3.5.4.1.

The need for a multiscale approach stems from the fact that the performance measures depend on TH behavior within a few meters of the emplacement drifts and also on thermal and TH behavior on a repository (or mountain) scale. A single numerical model cannot readily incorporate the required range of scales, for locations throughout the repository, without involving an unfeasible number (millions) of grid blocks. Consequently, a procedure has been developed for estimating the results that would be obtained using a full-scale, three-dimensional repository model with drift-scale resolution (i.e., millions of grid blocks) incorporating DKM for radiation, convection, and conduction.

A possible approach to the multiscale prediction problem would be to embed a three-dimensional drift-scale model with a relatively fine mesh into a three-dimensional repository-scale model with a coarse mesh. This approach is also too computationally intensive for the required number of cases. The multiscale approach presented subsequently combines one-, two-, and three-dimensional thermal-conduction-only models (T-models) and TH models at different scales to estimate the required performance measures.

3.5.1.2 Calculated Performance Measures

The multiscale approach combines one-, two-, and three-dimensional drift-scale T models and TH models with a conduction-only three-dimensional mountain-scale model (Figure 3-30). Output from this system provides estimates for the time evolution of the performance measures of the engineered barrier system summarized in Figure 3-30. These measures are used by TSPA-VA to estimate waste package corrosion rates, waste-form dissolution rates, and transport of radionuclides through the engineered barrier system.

The use of conduction-only models will introduce small errors in the abstracted performance measures. The magnitude of these errors can be estimated by comparison of abstracted results with direct simulations. Where possible, conduction-only models are used to calculate temperature differences instead of absolute temperatures; this minimizes the abstraction errors.

The TH performance measures (Table 3-9) are provided to TSPA-VA for various combinations of the following:

- Different locations in the repository
- Variations in heat production corresponding to different waste package designs and types of waste such as CSNF vs. defense HLW, CSNF age and burnup, waste package spacing, and sequencing of waste-package types in the emplacement drifts
- Design options such as an engineered backfill emplacement drift
- Design studies including line-loading design.

The TH performance measures are also provided for testing sensitivity of the TSPA-VA to variations such as the following:

- Alternative thermal and hydrologic properties
- Alternative distributions of infiltration flux, including the influence of climate change
- Alternative conceptual models of fracture–matrix interaction (e.g., comparing ECM with DKM results)
- Alternative conceptual models of heat-flow conditions at the water table, (e.g., a fixed temperature vs. explicit representation of heat loss to the SZ).

Given the number of required implementations of the calculation procedure for TSPA-VA performance measures, the multiscale approach was developed to efficiently incorporate as much detail as is computationally feasible.

3.5.1.2.1 Multiscale Submodel Nomenclature

Four different submodel types are used by the TH multiscale modeling and abstraction method:

- Smeared-heat source, Mountain-scale Thermal conduction-only (SMT) model
- Smeared-heat source, Drift-scale, Thermal conduction-only (SDT) model
- Line-averaged heat source, Drift-scale, TH (LDTH) models that use the DKM conceptual model
- Discrete-heat source, Drift-scale, Thermal conduction-only (DDT) models.

These submodels are defined and discussed in the following subsections (see Table 3-10). In addition, smeared-heat source, Drift-scale, TH (SDTH) model has been used during the course of model-abstraction testing.

The SDTH model is used to determine thermal conductivity relationships for the conduction-only models. With this and the SDT submodel, a thermal conductivity as a function of temperature is developed to estimate the affect of drying on the heat transfer rate by conduction.

3.5.1.3 Location-Specific Data for Calculation of TSPA-VA Performance Measures

Drift-scale model calculations are made throughout the repository area (Table 3-11) in either a slightly irregular 3 × 5 grid or a uniform 5 × 7 grid (c). The 3 × 5 grid with 15 locations is used for sensitivity analysis (Buscheck et al. 1997a, pp. 2-5 through 2-14). The 5 × 7 grid with 35 drift locations is used for the TSPA-VA TH predictions. The vertical hydrostratigraphy for all of these locations, including the elevations of unit contacts, and unit properties, is consistent with the UZ site-scale model (Bodvarsson et al. 1997).

Local infiltration flux is taken from the Flint et al.(1996a) infiltration map shown in Figure 3-31 (DTN GS96090831221.003, Qualified). For the 3 × 5 grid, an exponential area-weighting function is used with a length scale of 100 meters; for the 5 × 7 grid, the length scale is 50 meters (horizontal). The weighting function is used to ensure that the most appropriate infiltration rate boundary condition (taken from the infiltration map) is assigned to the specified drift-scale model location. It is necessary to preserve the variability in infiltration rate by appropriate weighting of neighboring data points (with respect to a drift-scale model location) taken from the infiltration map. The assumed infiltration flux values for the 5 × 7 grid are given in Table 3-12.

3.5.1.4 Description of Submodels Used in TH Multiscale Modeling and Abstraction Method

3.5.1.4.1 Smeared-Heat-Source, Mountain-Scale, Thermal Model

The three-dimensional SMT submodel enables the TH multiscale modeling and abstraction method to capture the influence of surface topography and edge-cooling effects on repository temperature. Temperature predictions are then used for interpolating other performance measures such as waste package relative humidity for waste packages located near repository edge. The SMT model also captures the influence of the thermal-property distribution in the mountain on the overall temperature distribution. The specific SMT model input to the TH multiscale modeling and abstraction method is the repository host-rock temperature T_{rep} (SMT). Because the SMT results are predicted with a thermal-conduction model, temperatures above the boiling point will be overpredicted relative to those predicted by a TH model.

Transient, three-dimensional, conduction-only problems can be solved readily by NUFT, permitting the use of fine lateral and vertical grid-block spacing in the repository area. At the repository edges, a lateral grid-block spacing of 15 meters is used. In the vertical interval that corresponds to the dryout zone in TH models, a vertical grid-block spacing of about 4 meters is used.

The repository is represented as a rectangular approximation of the actual shape (Figure 3-31c). The long axis of the repository is oriented three degrees from the north. The SMT model assumes the north–south length of the repository to be 2912 meters, which is obtained from the product of 104 emplacement drifts times the drift spacing of 28 meters. The SMT model assumes the east–west width of the repository to be 1109 meters, which is obtained by dividing the area of the overall heated repository footprint (3.23 km^2 or 798 acres) by 2912 meters.

For an areal mass loading (AML) of 85 MTU/acre (calculated on the basis of CSNF) and 63,000 MTU of CSNF, the repository area is calculated to be 741 acres(3.00 km^2), which is 7.5% less than the 798-acre repository area assumed in the SMT model. However, four to five of the 104 emplacement drifts are left empty; thus about 4% of the repository drifts are not directly heated by waste packages. Note that the bulkheads that will separate the emplacement drifts from the perimeter drifts are located about 30 meters from the outermost waste packages at the eastern and western ends of the emplacement drifts. Heat-transfer mechanisms, such as the cold-trap effect (Buscheck 1996; Buscheck et al. 1997b) and thermal radiation will efficiently distribute the decay heat well beyond the outermost waste packages. The assumption is effectively made that decay heat is axially spread 18 meters beyond the outermost waste packages at either end of

the drifts, thereby increasing the effective heated length of the emplacement drift by 36 meters. When these adjustments are made, the heated footprint of the repository becomes 798 acres, and the effective AML becomes 78.9 MTU/acre.

The SMT model represents the 1.6% south-to-north dip of the repository. In the east–west direction, the repository is represented as being horizontal. For the actual repository, the eastern and western boundaries have the same elevation, whereas the center of the repository (in the east–west direction) is elevated by about 3 meters relative to the eastern and western edges. The small rise at the center of the repository is neglected in the SMT model.

The numerical grid for the SMT consists of three concentric nests of grid blocks. The preprocessor YMESH determines the areal dimensions of the grid blocks on the basis of user-specified dimensions for each of the nests. YMESH determines the vertical grid-block spacing on the basis of user-specified criteria and honoring the unit contacts in the UZ site-scale model. The vertical spacing criteria are specified for each nest. The objective is to provide fine spatial resolution in the repository area, with the grid refinement increasing in proximity to the repository edges. Because of the large number of model units (Figures 3-32 through 3-38), relatively fine vertical grid refinement occurs over the entire UZ, particularly within the Paintbrush Tuff (ptn21–ptn25) units.

Thermal-loading conditions of the reference 85-MTU/acre repository are represented as a uniform, 4.52-meter-thick, smeared-heat source, which is a blend of the heat-decay curves (refer to Section 3.5.3 and Figure 3-41) for the entire waste inventory.

The dependence of rock thermal conductivity K_{th} on liquid-phase saturation S_{liq} is approximated by correlating temperature in the conduction-only-model to S_{liq} in a corresponding SDTH model and developing a corresponding functional relations between K_{th} and temperature in the conduction-only-model. This K_{th} vs. T relationship in the T-model mimics the K_{th} vs. S_{liq} in the TH model. This effect is particularly important in the lower lithophysal tsw35 model unit because of the relatively low value of dry thermal conductivity in that unit.

The surface topography, hydrostratigraphy (including all of the model units), and temperature boundary conditions of the UZ site-scale model (Bodvarsson et al. 1997) are incorporated in the SMT model. The thermal load for the total waste inventory (63,000 MTU of CSNF; 4667 MTU of HLW; 2333 MTU of separate-disposal DOE SNF waste) is uniformly distributed over a heated repository footprint of three to three and a quarter square kilometers.

The three-dimensional SMT submodel (Figure 3-30d) incorporates the following processes, conditions, and assumptions:

- Three-dimensional mountain-scale heat flow in the UZ and in the upper 1,000 meters of the SZ.
- Convective heat flow is driven by regional groundwater flow in the upper 1,000 meters of the SZ. For the TSPA-VA calculations, the influence of regional groundwater flow on heat flow is assumed to be negligible.

- Topography, stratigraphy, thermal properties, temperature boundary conditions, and initial temperature are consistent with the UZ site-scale model (Bodvarsson and Bandurraga 1996; Bodvarsson et al. 1997). Because the SMT model extends below the lower boundary of the UZ site-scale model, it is necessary to vertically extrapolate the temperature distribution from the UZ site-scale model below the water table. This is based on the slope of the geothermal gradient of the lower most units in the UZ flow site-scale model.

- The influence of dryout on rock thermal conductivity K_{th} is approximated with the use of a K_{th} vs. temperature relations. The dependence of K_{th} on liquid-phase saturation S_{liq} is approximated by correlating temperature computed with a one-dimensional SDT model, with S_{liq} in a corresponding one-dimensional SDTH model, and developing a functional relations between K_{th} and temperature predicted by the SDT model. The K_{th} vs. T relations in the SDT model mimic the K_{th} vs. S_{liq} in the SDTH model.

- The vertical and areal geometry of the reference 85 MTU/acre repository design is closely approximated in the SMT.

- Homogeneous (lateral) thermal properties are assumed within each hydrostratigraphic unit. However, the properties vary from unit-to-unit. This assumption is consistent with the assumption of lateral homogeneous hydologic properties applied in other models for TSPA-VA.

- Thermal-loading by the reference 85-MTU/acre repository is represented as a uniform, 4.52-meter-thick, smeared-heat source, based on a composite of the decay curves for the entire waste inventory. The SMT assumes the same heat-producing area as that in the reference repository.

- Mountain-scale, buoyant, gas-phase convection in the UZ does not significantly influence the temperature distribution. This assumption is least well suited to repository edge locations where buoyant gas-phase convection is most likely to be significant. This assumption will be reconsidered using a mountain-scale TH model in the TH multiscale modeling and abstraction method used in future abstraction and testing analyses for the license application.

- Mountain-scale condensate flow in the UZ does not significantly influence the temperature distribution. Using the abstraction methodology, vertical flow of condensate is simulated explicitly. However, the lateral component of this flow is not, and it may be significant at repository edge locations. This assumption will be reconsidered using a mountain-scale TH model in the TH multiscale modeling and abstraction method used in future abstraction and testing analyses for the license application.

- Mountain-scale, buoyant, liquid-phase convection in the SZ does not significantly influence the temperature distribution. Heat flows from the unsaturated zone to the saturated zone by conduction and convection heat transfer processes. Convection heat

transfer in the SZ includes regional groundwater flow as well as a natural convective component initiated by repository heating. The SMT model includes the component of heat transfer into the SZ by conduction-only. This assumption provides an upper bound on temperature at the UZ and SZ interface since heat removal by convection at this location is neglected. In contrast, a constant temperature interface provides a lower bound on the temperature.

- The influence of regional groundwater flow does not significantly influence the temperature distribution. As in the previous assumption, including only heat conduction from the UZ-SZ interface provides an upper bound on the temperature at this location. As indicated in Ho et al. 1996, pp. 7-5 and 7-6, the heat transfer below the water table is primarily dominated by thermal conduction because of the low groundwater velocities.

The SMT model was selected because its computational economy allows for the use of fine lateral and vertical grid-block spacing in the repository area. At the repository edges, a lateral grid-block spacing of 15 meters was used. In the vertical interval that corresponds to the dryout and heat-pipe zones in the TH models, a vertical grid-block spacing of about 4–8 meters was used. Thus, relatively fine gridding is used to capture the influence of edge-cooling effects and the temperature distribution in the vertical interval of what would be the dryout and heat-pipe zones. If mountain-scale, buoyant, gas-phase convection significantly affects the temperature distribution in the repository, it would be useful to use a smeared-heat source, mountain-scale, thermal-hydrologic (SMTH) model rather than the SMT model, which cannot capture convective heat-flow effects in the UZ. This analysis is to be considered further in future abstraction and testing activities for the license application.

3.5.1.4.2 Smeared-Heat-Source, Drift-Scale, Thermal Model

The one-dimensional SDT submodel (Figure 3-30a) incorporates the following processes, conditions, and assumptions:

- One-dimensional vertical heat flow in the UZ is equivalent to that in the LDTH (described in the next section) and DDT (described in Section 3.5.1.4.4) models.

- For TSPA-VA TH predictions, the water table is assumed to be a constant temperature boundary, consistent with the UZ site-scale flow model (Bodvarsson and Bandurraga 1996; Bodvarsson et al. 1997). (However, heat flow by conduction-only below the water table is included in the SMT described previously. This model and the LDTH are used for hydrology corrections to the SMT model. The SMT model previously described provides the starting point temperature upon which all corrections are made.)

- Local topography, stratigraphy, thermal properties, temperature boundary conditions, and initial temperature are consistent with the UZ site-scale model (Bodvarsson and Bandurraga 1996; Bodvarsson et al. 1997). The SDT submodel calculations are made throughout the repository area with a uniform 5×7 grid (Figure 3-31 and Table 3-11). Figures 3-32 through 3-38 and Table 3-11 give the vertical hydrostratigraphy for the 35 drift-scale model locations.

- The thermal properties within each hydrostratigraphic unit are homogeneous.

- The thermal load is represented as a 4.52-meter-thick, smeared-heat source, just as in the SMT model; however, the SDT model does not use the same heat-of-decay curve as does the SMT model. It smears the heat from the seven waste package drift-scale model (see Section 3.5.3).

- The smeared-heat source in the SDT model uses a heat-of-decay curve that is an areal average of the heat-of-decay curves used in the LDTH and DDT models. The SDT, LDTH, and DDT models all assume the same seven waste package types that are described in Figure 3-39.

- AMLs of 85, 56.67, and 42.5 MTU/acre are assumed for SDT submodel calculations. The two smaller loads are used to represent cooler areas, such as those near the edges of the repository.

The primary role for the SDT submodel in the multiscale approach is to provide a functional relationship between repository host-rock temperature predicted with the SDT submodel and the perimeter-averaged drift-wall temperature predicted by a LDTH model. This functional relationship allows estimation of the perimeter-averaged drift-wall temperature T_{dw}(LMTH) using the calculated conduction-only, mountain-scale temperature T_{rep}(SMT).

The SDT submodel input to the TH multiscale modeling and abstraction method is repository host-rock temperature T_{rep}(SDT). The SDT submodel calculations are made in parallel with the LDTH model calculations. The LDTH is described in the next section.

3.5.1.4.3 Line-Averaged-Heat-Source, Drift-Scale, Thermal-Hydrologic Model

The two-dimensional LDTH submodel (Figure 3-30b) incorporates the following processes, conditions, and assumptions:

- One-dimensional vertical heat flow in the UZ is equivalent to that of the SDT and DDT models.

- For TSPA-VA TH predictions, the water table is assumed to be a constant-temperature boundary, consistent with the UZ site-scale model (Bodvarsson and Bandurraga 1996; Bodvarsson et al. 1997). (However, heat flow by conduction-only below the water table is included in the SMT described previously.) This model and the LDTH are used for hydrology corrections to the SMT model. The SMT model previously described provides the starting point temperature upon which all corrections are made.

- Point-load and line-load designs are considered by using different values for the linear power density of the line-heat source and different values of drift spacing. This is a direct result of waste package spacing along the emplacement drift. Point loaded waste packages are widely spaced (lower linear power density), line-loaded waste packages are very nearly end-to-end (higher linear power density).

- At the drift scale, two-dimensional heat flow (as well as mass flow) is represented in the near-field rock and in the emplacement drifts. Heat flow in and near the drifts is primarily radial.

- The cross-sectional, two-dimensional geometry of the emplacement drifts is represented, including the invert, waste package, and the open drift below, above, and to the side of the waste package. For drift backfill scenarios, the open space in the drift is partially filled with a uniform, porous material. The grid for the model with backfill has more resolution (increased the number of grid blocks by three laterally and by four vertically) in the drift than the model with no backfill in order to better represent the influence of seepage and capillary-driven wicking in the backfill (see Section 3.6.3 for backfill results).

- As demonstrated in an earlier study (Buscheck 1996, p. 1.10-26), a circular waste package in a circular drift opening can be accurately represented by a square waste package in a square drift, insofar as prediction of the key performance measures, provided that the circular cross-sectional areas are equal to the equivalent square cross-sectional areas. Accordingly, for the LDTH submodels, the circular geometry of the waste package and the drift is approximated by rectilinear geometry (Figure 3-40). The drift is represented as being 4.52 meter × 4.52 meter, and the waste packages are represented as 1.445 meter × 1.445 meter in cross-section. The invert is assumed to occupy ~11% of the drift cross-section. Note that the same cross-sectional geometry is used for the LDTH and DDT models.

- Radiative heat transfer is represented between all surfaces in the emplacement drifts, resulting principally in heat transfer between the waste packages and adjacent surfaces. (see Figure 3-40)

- Local topography, hydrostratigraphy, thermal properties, hydrologic properties, boundary conditions such as temperature, air mass fraction, and gas-phase pressure (T, $X_{air,gas}$, P_{gas}), and initial temperature are consistent with the UZ site-scale model (Bodvarsson and Bandurraga 1996; Bodvarsson et al. 1997).

- Local infiltration flux is taken from the Flint (1996) infiltration map (Table 3-12).

- The thermal and hydrologic properties within each hydrostratigraphic unit are homogeneous.

- The LDTH model uses a heat-source decay curve that is an average of the decay curves for the seven individual waste packages represented in the DDT model. In other words, the LDTH model smears the heat output from a conduction-only model, which uses discrete heat sources, into a line-averaged heat source. The SDT, LDTH, and DDT models all assume the same seven waste-package types described in Figure 3-39.

- The DKM is used to represent fracture–matrix interaction.

- AMLs of 85, 56.67, and 42.5 MTU/acre are assumed for LDTH submodel calculations. The two smaller values are used to represent cooler areas (e.g., near the edges of the repository).

One of the primary roles for the LDTH model in the TH multiscale modeling and abstraction method is to provide a functional relationship between repository host-rock temperatures predicted with a thermal-conduction-only model and the perimeter-averaged drift-wall temperature predicted by a TH model. This relationship allows the mapping of the LDTH perimeter-averaged drift-wall temperature T_{dw}(LDTH) onto the SMT-predicted repository host-rock temperature T_{rep}(SMT). This approximates a drift-wall temperature prediction from a mountain-scale model with a finely resolved, line-averaged heat source T_{dw}(LMTH), which can be readily computed for locations throughout the repository area. It includes the hydrology of the system indirectly through the functional relationship developed with the LDTH and SDT submodels. The T_{dw} (LMTH) is an example of an abstracted result from the TH multiscale modeling and abstraction method.

Another role for the LDTH model is to provide a functional relation between the drift-wall temperature T_{dw}(LDTH) and other TH conditions in the NFE, including the perimeter-averaged relative humidity RH_{dw}(LDTH) at the drift wall, the liquid-phase flux three meters above the drift, and the liquid-phase saturation in the invert $S_{liq,inv}$(LDTH).

The LDTH submodel inputs to the TH multiscale modeling and abstraction method include the following:

- Perimeter-averaged, drift-wall temperature T_{dw}(LDTH)
- Perimeter-averaged, drift-wall relative humidity RH_{dw}(LDTH)
- Perimeter-averaged, drift-wall liquid-phase saturation S_{liq}(LDTH)
- Liquid-phase flux three meters above the drift q_{liq}(LDTH)
- Liquid-phase saturation in the invert $S_{liq,inv}$(LDTH).

The LDTH submodel calculations are made in parallel with the SDT calculations.

3.5.1.4.4 Discrete-Heat-Source, Drift-Scale T Model

The three-dimensional conduction-only DDT model (Figure 3-30c) incorporates the following processes, conditions, and assumptions:

- One-dimensional vertical heat flow in the UZ is equivalent to that of the SDT and LDTH models.

- Point-load (reference design) and line-load (section 3.6.4) designs are considered, as are backfill and no-backfill (reference design) scenarios.

- At the drift scale, three-dimensional heat flow is represented in the near-field rock and in the emplacement drifts. For the point-load design, heat flow in and near the drifts is spherical at early time, becoming more radial at later time. For the line-load design,

heat flow in and near the drifts is mostly radial due to the proximity of the waste packages to each other in the drift (very closely spaced).

- The full three-dimensional geometry of the emplacement drifts is represented, including the invert; waste packages; the open drift lying below, above, and to the side of the waste packages; and the open drift lying axially between waste packages (Figure 3-39 shows a plan view of the emplacement drift). For drift backfill scenarios, the open space in the drift is partially filled with a uniform, porous material.

- The circular cross-sectional geometry of the waste package and drift are approximated with squares having the same cross-sectional areas as their circular counterparts (Figure 3-40). The cross-sectional drift geometry is the same as that discussed previously for the LDTH sub-models.

- Radiative heat transfer is represented between all surfaces in the emplacement drifts, resulting principally in heat transfer between the waste packages and adjacent surfaces.

- Local topography, hydrostratigraphy, thermal properties, temperature boundary conditions, and initial temperature are consistent with the UZ site-scale model (Bodvarsson and Bandurraga 1996; Bodvarsson et al. 1997). For the preliminary base-case and base-case TSPA-VA EBS TH predictions, DDT model calculations are conducted for the center location of the repository, which is the l4c3 location in the 5×7 grid (Table 3-11) for the cases with no backfill. For the cases with engineered backfill, the DDT model calculations were conducted for the l5c2 location of the 5×7 grid. The grid for the model with backfill has more resolution in the drift than the model with no backfill.

- The thermal properties within each hydrostratigraphic unit are homogeneous.

- The DDT model discretely represents decay-heat output from seven waste packages (Figure 3-39). The DDT represents six full waste packages and two half waste-packages. The SDT, LDTH, and DDT models all assume the same seven waste-package types, as described in Figure 3-39.

- Repository AML of 85 MTU/acre is assumed for the DDT submodel calculations.

An important role for the DDT model in the multiscale TH modeling approach is to represent the drift-wall temperature differences that occur between specific waste-package locations (ΔT_{dw}), which are defined relative to the average drift-wall temperature along the drift T_{dw} (LMTH). Another role is to determine the temperature difference between the waste package and the average drift-wall temperature ΔT_{wp}.

The DDT submodel inputs to the TH multiscale modeling approach include and abstraction method include the following:

- Waste-package-location-specific temperature differences ΔT_{dw} from the average drift-wall temperature along the drift

- Waste-package-location-specific temperature difference ΔT_{wp} between the waste package and the average drift-wall temperature along the drift.

These quantities are necessary to determine the waste package variability.

The DDT (conduction-only) model determines drift-wall and waste-package temperature differences, as determined from comparison with a drift-scale model including directly the hydrology of the system (i.e., a DDTH model, Busheck et al. 1997a, p. 3-9.) The DDT model predicts slightly higher absolute drift-wall and waste-package temperatures than does the DDTH model, but the two models produce very similar temperature differences at each of the eight waste package locations. This is important because it requires several days to conduct a single DDTH calculation on a Sun Ultra2 Sparc workstation, whereas it takes only about one hour to conduct the corresponding DDT calculation.

The differences in temperature at hotter and cooler locations along the emplacement drift are related to the heat-flux distribution, which is controlled by thermal radiation for the no-backfill case or by thermal conduction for the backfill case. Advective heat transfer driven by TH behavior in the host rock has little effect on axial temperature variation in the drift. In other words, TH processes in the host rock do not contribute significantly to equalization of axial temperature variations in the drift (Ho and Francis 1996). This concludes the discussion of the modeling approach used to generate in-drift thermodynamic variables. Inputs to these submodels include property specifications (hydrologic and thermal) as well as repository design criteria. These are the topics of the next two sections.

3.5.2 Development of Thermal-Hydrologic Parameter Distributions and Uncertainties

Thermal-hydrologic model analyses for TSPA-VA require inputs from other process-level model abstraction and testing activities. *Of particular importance to TH are the hydrologic property and infiltration rate uncertainties and other variabilities (such as climate change) developed within the UZ flow tasks (see Chapter 2, TSPA-VA Technical Basis Document)* for the viability assessment. Thermal-hydrologic "uncertainty" is incorporated into TSPA-VA through the use of a hydrologic property set determined to be more appropriate for the measured temperature results of the single-heater test. This property set is governed by rewetting characteristics of fractures and matrix somewhat different than those applied to the hydrologic property sets developed for TSPA-VA.

The following section will discuss the hydrologic properties, thermal properties, and in-drift material properties such as concrete invert and liner materials applied to the TH analyses. It describes the base-case set of thermal and hydrologic properties used in the analysis. Section 3.6.2 of this chapter indicates other hydrologic property sets used in sensitivity studies for TH. Each of the property sets used in the viability assessment is described in detail in Chapter 2 on UZ flow models for TSPA-VA Technical Basis Document. The additional property set used to represent rewetting uncertainty characterized by TH is the "thermal-hydrologic property set." It is described in Section 3.6.2.

The "thermal-hydrologic property set" was developed to provide a better match with the results of the single-heater testing temperature data. This property set is similar to the base case, with the major exceptions occurring in the rate of rewetting parameters applied to the host-rock units (tsw4, tsw5, and tsw6 in the site-scale UZ flow model) and in the matrix diffusivity parameter of the lowermost Topopah Spring hydrogeologic model units (tsw6 and tsw7 in the site-scale UZ flow model). The rewetting parameters include fracture van Genuchten alpha (α_f) and the matrix diffusivity parameters such as matrix permeability (K_m) and matrix van Genuchten alpha (α_m). These parameters govern the extent and duration of a superheated dryout zone. If the inversion model prediction of α_f is too small, capillarity in fractures will govern rewetting forces and limit the extent and duration of dryout formation during a heating process. If the matrix diffusivity is too large, a superheated region may not form or may be limited in extent. Therefore, in addition to larger fracture van Genuchten alphas in the repository host units, the "thermal-hydrologic property set" also specifies less variability in matrix permeability values in the host rock. This requires that the lower hydrogeologic model unit, tsw7 (Tptpv), has a matrix permeability identical to that in the tsw4 (Tptpmn) model unit. Therefore, it is effectively decreased from the base-case value listed in Table 2-20 in Chapter 2 of the TSPA-VA Technical Basis Document. Matrix van Genuchten alphas in the tsw6 (Tptpln) and tsw7 model units are increased, thus decreasing overall the matrix diffusivity of these units. This discussion is clarified by noting that the matrix diffusivity is proportional to the following:

$$D_{imb} \propto \frac{K_m}{\alpha_m} \tag{3-16}$$

Subsequently, the matrix diffusivity of the tsw6 and tsw7 model units is identical to tsw4 model unit. In this thermal-hydrologic property set the rate of rewetting in the repository host units is not dominated by capillary forces. The results of this analysis are shown in Section 3.6.2.2.

However, in Approach and Implementation of Abstraction for Thermal Hydrology, Section 3.4.5, the base-case property set was shown to compare reasonably well to the single-heater test results, when applied in a DKM conceptualization of the single-heater test geometry. Consequently, this thermal and hydrologic property set was chosen as the base case (when compared to the preliminary base case) based on these results.

3.5.2.1 Hydrologic Properties

The base-case property set includes five independently calibrated models used to address both hydrologic property and infiltration rate uncertainty. The hydrologic property uncertainty addressed in the base-case property set is the capillary characteristic of the fracture, α_f, and the fracture-matrix coupling strength, X_{fm} (see Section 2.4.3.1 in Chapter 2 of the TSPA-VA Technical Basis Document). The fracture-matrix coupling strength is a calibration variable with three possible values depending on geologic unit. The fracture α_f parameter includes a range of uncertainty for the base-case models. This parameter is the van Genuchten alpha parameter characterizing the capillary pressure in the fractures. *In all of the TH analyses, it is tacitly assumed that the van Genuchten representation applies to the fractures as well as to the matrix rock.* The fracture alpha parameter controls the wicking potential in the fractures. The base-case hydrologic property sets consider a minimum, mean, and maximum fracture alpha range. A

minimum fracture alpha drives increased wicking in the fractures. This characteristic parameter is especially important during the rewetting processes that occur after the repository cools and the dryout zone begins to return to a near ambient state. The rate at which rewetting occurs in the dryout zone is influenced by this parameter. In addition to hydrologic property uncertainty, infiltration rate uncertainty is also addressed in the base-case models; the present day infiltration rate, denoted as I, contains uncertainty in the range of I/3 to I*3. (The present day infiltration rate divided by three or multiplied by three.) The potential ranges in infiltration rate are constrained by the current natural geothermal gradient measured in the UZ at Yucca Mountain.

The base-case property set information is given in Table 3-3 and is repeated here for convenience. For Base-Case, mean α_f, the DTN is LB971212001254.001; for Base-Case, min α_f, I/3, the DTN is LB971212001254.002; for Base-Case, min α_f, I*3, the DTN is LB971212001254.003; for Base-Case, max α_f, I/3, the DTN is LB971212001254.004; and for Base-Case, max α_f, I*3, the DTN is LB971212001254.005. Each of the five base-case property sets is unqualified data.

Since most of the details related to the hydrologic property sets and scoping sensitivities with respect to individual hydrologic parameters are found in Chapter 2 of the TSPA-VA Technical Basis Document, we will limit our discussion associated with hydrologic properties to potential TH response only. This includes rewetting characteristics of a dryout zone, bulk fracture permeability, and fracture van Genuchten alpha, in particular, at the repository horizon.

The potential repository horizon falls within the Topopah Springs Middle Nonlithophysal (Tptpmn), Lower Lithophysal (Tptpll), and the Lower Nonlithophysal (Tptpln) geologic units. In terms of the site-scale UZ flow model units, the potential repository horizon falls within the following hydrogeologic unit definitions: tsw4, tsw5, and tsw6, respectively. The majority of the repository occurs within the tsw5 hydrogeologic unit. Portions of the northeast repository fall within the tsw4 hydrogeologic unit while portions of the southwest corner fall within the tsw6 hydrogeologic unit. Since these hydrogeologic units are of particular importance to the TH analyses, both abstraction results and model testing, they are listed for each of the base-case property set models in the following tables. For a complete listing of all remaining hydrogeologic properties applied to the base case for TSPA-VA, refer to Tables 2-18 through 2-22 in Chapter 2 of the TSPA-VA Technical Basis Document. Table 3-13 displays the repository host-rock properties for the mean fracture alpha, nominal infiltration rate case.

M or F in the material name stands for matrix or fracture, respectively. The fracture permeability (both horizontal and vertical) listed is the bulk fracture permeability. The bulk permeability is the product of the intrinsic fracture permeability and the fracture porosity. S_r and S_{ls} are defined as the residual and matrix satiation saturation parameters. It is noted that for DKM simulations, the matrix satiation saturation is specified as 1.0. The G-ECM simulations redirect flow into fractures with the use of a specified average matrix satiation saturation value (refer to Section 3.4.2). As matrix saturation rises to the satiation saturation value, water is diverted into fractures. This matrix satiation saturation is not required in the DKM since there are no capillary-pressure and thermal-equilibrium requirements between the fractures and the matrix rock. The *(f(Sup)* in Section 3.4.2.3) term is not required for G-ECM simulations; it is used only in the DKM simulations for coupling between fracture and matrix rock. It is assumed that

quality status of the hydrologic property data, developed in Chapter 2, applies to the TH analyses as well. Simply put, this infers that the hydrologic properties developed to describe ambient flow processes can also be applied to thermally driven flow processes. This assumption is the very reason for the development of the "thermal-hydrologic property set."

The remaining infiltration-rate and property-set data for the base-case model at the repository horizon are given in Table 3-14 through Table 3-17.

The tables given above indicate the uncertainty in the ground-surface infiltration rates as well as fracture hydrologic properties (α_f, X_{fm}) at the potential repository horizon units. Tables 2-18 through 2-22 in Chapter 2 of the TSPA-VA Technical Basis Document contains hydrologic property data for each of the hydrogeologic units applied in the TH model domains. In addition to the hydrologic property specifications and uncertainties, TH models also require thermal properties (grain density, thermal conductivity, specific heat, and gas-phase tortuosity) as TH models also solve for the conservation of energy equation.

3.5.2.2 Thermal Properties

Thermal properties used in all of the TH analyses (both base case models and testing models) are given for all model units in Table 3-18. It is assumed that uncertainty associated with thermal properties is much less than that associated with hydrologic-properties, in particular, fracture hydrologic properties. Thermal properties do not in general vary by orders of magnitude as their measurement techniques are well founded. As an example of measured variability of the thermal conductivity, the experimental value of the thermal conductivity applied in the site-scale model unit tsw2 (Tptrn) is 1.62 ± 0.12 (W/m-K). Subsequently, only the mean values obtained from experimental measurements of thermal properties are applied to the TSPA-VA TH analyses. Thermal properties such as wet and dry thermal conductivity, rock grain density, rock grain specific heat, and tortuosity coefficient are listed for each of the hydrogeologic units applied in the site-scale flow model and also applied in TH models. The thermal property data are found in DTN: SNT05071897001.002. This technical data information file (TDIF) contains detailed information as to the sources of data and the development for its use in the models for TSPA-VA. The developed thermal data are not qualified data. The developed thermal property data listed in this TDIF are for TH as well as conduction-only models.

The base-case set of thermal properties is compiled from recent experimental data obtained by the project (Brodsky et al. 1997; Flint 1996), recent correlated data and models (Rautman and Engstrom 1996a; Rautman and Engstrom 1996b, Engstrom and Rautman 1996; Rautman 1995), and the Reference Information Base (RIB) (U.S. DOE 1995). Experimental data are selected first. Where experimental data are not available, correlated data or models are used. The information indicating which of the following applies: experimental data, correlated data, or other models is given in detail in DTN: SNT05071897001.002.

3.5.2.3 In-Drift Material Properties

Thermal and hydrologic properties have also been obtained for the concrete liner and invert material inside the emplacement drift. Thermal properties for the concrete materials in the drift are given in Table 3-19, (taken from CRWMS M&O 1997d, pp. 11):

Hydrologic data for concrete are given in Table 3-20. The table includes both fracture and matrix properties. The hydrologic data for concrete are unqualified data and are developed from the following sources. The ground-support-materials report (CRWMS M&O 1997c, pp. 6 of 74 and 38 of 74) indicates that the emplaced concrete is to have a water/cement ratio of 0.4 and a maximum aggregate size of 3/4 inches (TSw tuff to be used as the coarse aggregate). It is indicated that standard, good-quality concrete has a permeability of 1.0×10^{-10} cm/s (1.0×10^{-19} m^2) and that low-permeability concretes are an order of magnitude lower.

Mehta 1986 displays a plot of porosity as a function of water/cement ratio and hydration. For a water/cement ratio of 0.4 and 100% hydration, it shows a porosity of about 0.12. Jacobs et al. 1994, p. 90, table 2, show a porosity of 0.101 for a concrete with a water/cement ratio of 0.45.

Mehta also shows graphs of permeability vs. water/cement ratio and permeability vs. porosity. A water/cement ratio of 0.4 and a porosity of 0.1 are at the extreme of the plotted range, and the permeabilities are too low to read with any accuracy. They show $k < 1.0 \times 10^{-11}$ cm/s = 1.0×10^{-20} m^2. (According to the ground-support-materials report, the strength and durability of concrete both increase as water/cement ratio and permeability decrease, which is why they are specifying low water/cement and low permeability.) Jacobs et al. (1994), p. 90 table 2, shows a permeability of 2.0×10^{-19} m^2 for their water/cement ratio of 0.45 concrete --and reports a gas permeability even higher: 3.0×10^{-17} m^2. Fernandez et al. (1987), pp. G-3 and G-23, report tests of a water/cement ratio of -0.4 concrete, and they give a permeability of 3.88×10^{-19} m^2 (average of 6 samples). It seems reasonable to assume the lower value of 1.0×10^{-20} m^2. Fortunately, since water flow and transport will probably be primarily through gaps and cracks (see below) and not through the matrix, this assumption should not dictate the flow processes greatly.

Jacobs et al. (1994) and Fernandez et al. (1987) both present saturation curves for their concretes. Fernandez even give van Genuchten parameters for theirs: $\alpha = 8.14 \times 10^{-4}$/m, $\beta = 1.36$, $S_r = 0.0324$ (average of 6 samples). Using the relation $d = 28/\psi$, where d is pore diameter in microns and ψ is suction head in meters, this saturation curve represents a pore-size distribution that starts at about 300 nm and goes down from there. This agrees with Mehta, who indicates that well-hydrated concrete typically has pores between 10 and 100 nm. The Fernandez et al. (1987) saturation curve has most of its pores in about the right range, but it also has a lot of very small pores—about 30% are less than 1 nm, which is not physical (though such high capillary pressures may not represent physical pore sizes, but rather an adsorbed or bound water layer to the concrete solid). The Jacobs et. al (1994) paper shows significantly lower capillary pressures, corresponding to significantly larger pores. Most of their pores are in the 10 -100 nm range, but with a substantial fraction going up to tens of microns. A rough fit of their saturation curve to a van Genuchten curve results in $\alpha = 6.0 \times 10^{-3}$/m, $\beta = 1.5$, $S_r = 0$.

We have no real information about fracture properties in concrete. Note that there is a significant fracture contribution even initially (i.e., without cracking), because the liner and invert will be in segments, with gaps between them to accommodate the thermal expansion. Therefore, the fracture permeability is selected such that the bulk permeability is high enough so that water does not pond on top of it even when the water flux is at a maximum. The numbers in the table are based on a 1-mm fracture every meter, with the fracture beta equal to the matrix beta.

Finally, thermal properties for the waste package materials are given in Table 3-21 (taken from CRWMS M&O 1997d, p. 11).

This section described the thermal and hydrologic property inputs to the TH models used in TSPA-VA. The properties govern the flow of heat and fluids in the engineered barrier system and the natural geologic system as described by the models used to predict performance in the altered zone. The nature of the energy source imparted to Yucca Mountain must also be quantified in the TH models. Consequently, repository design-based inputs are also required. This is the topic of the next section.

3.5.3 Development of Repository Design Requirements

In addition to hydrologic and thermal property inputs in the TH models, criteria related to repository design is also required when performing post-waste-emplacement calculations. UZ flow model calculations determine the ambient flow conditions in the mountain. They result in steady-state gas pressure, liquid saturation, and geothermal temperature gradients from the ground surface to the water table. In fact, the ambient solutions are the initial conditions for the TH calculation. Since TH calculations determine the details of a thermal perturbation to the ambient system associated with a geologic repository, TH models require repository design information such as drift and waste-package spacing, waste package geometry and heat output, total waste stream, and the total repository thermal load. The thermal loading data required for the TSPA-VA analyses are documented in detail in DTN: SNT05071897001.004. The thermal loading data developed for the viability assessment thermal and TH calculations are unqualified data. The data given in this TDIF include both individual waste-package heat output and decay and repository-scale heat output and decay.

3.5.3.1 Base-Case Repository Design Description

The characteristics of repository thermal loading are described for both drift-and mountain-scale TH models currently being used in support of the TSPA-VA calculations. The differences in TH model scale are driven by specific needs of the TSPA-VA analyses. Some near-field models require waste-package surface and drift-wall-specific information such as waste-package temperature, waste-package relative humidity, and drift-wall temperature. This information is obtained from the models developed at the scale of the drift and the waste package as detailed previously in the TH multiscale modeling and abstraction process (see Section 3.5.1). Often, near-and far-field models require heat-driven behavior, at the scale of the entire repository, such as gas-phase flow rates and air mass fraction. This information is obtained from the TH model at the scale of the mountain. The overall (reference) repository design data implemented in the TH models of different scale are the following.

The total mass of commercial spent fuel to be emplaced at Yucca Mountain is 63,000 metric tons of heavy metals (CRWMS M&O 1997e, pp. 3-14). The average waste-package mass loading is obtained from CRWMS M&O 1997e, pp. 3-17. This mass includes several waste-package types of varying heat output (CRWMS M&O (1997b, pp. 45 and 55). The data obtained from CRWMS M&O (1997b) are subject to quality assurance controls and are to be verified. The expected number of commercial spent-fuel waste packages is about 7,650. Additional area is not expected to be needed for emplacing additional wastes such as HLW glass and DOE SNF. The

waste packages containing additional wastes are placed between the commercial spent-fuel waste packages, with a requirement of at least 1-meter separation between waste packages. The total emplaced mass of additional waste is 7,000 MTU of which 2,333 MTU is DOE SNF and 4,667 MTU is HLW glass. The number of additional waste packages expected to be emplaced in the repository is about 2,550. These waste packages include co-disposal (that is, two types of waste in the same disposal container) and separate (direct-)disposal waste packages. The co-disposal waste packages contain both HLW glass and DOE SNF; the direct-disposal waste packages contain only separate-disposal DOE SNF.

The reference design used in the TSPA-VA is for an 85-MTU/acre repository (CRWMS M&O 1997d, pp. 23), which is based on the commercial waste to be emplaced within the heated outline, or footprint, of the repository. Point-loading emplacement is specified, meaning that the spacing from package to package in an emplacement drift is approximately equal to the emplacement-drift half-spacing (from drift centerline halfway to the next drift centerline). A point-loaded drift segment is shown in Figure 3-39. All three waste-package types (commercial spent fuel, co-disposal, and direct-disposal) are illustrated in the figure. It is noted that the reference design data obtained from CRWMS M&O (1997d) are unqualified.

The reference-repository design specifies that the emplacement drifts contain no engineered backfill. The waste packages are placed on a pedestal on top of a concrete invert floor (concrete segments put in the bottom of the round emplacement drift to provide a level floor). The TH calculations for the TSPA-VA base case use these design conditions.

Enhanced repository designs include use of backfill and drip shields either directly on the waste packages or on top of the backfill material. Additional options include ceramic coatings on the waste packages. These options are expected to reduce the amount of liquid water in contact with the waste package. The presence of backfill also reduces relative humidity for a longer period of time after waste emplacement. In addition to the reference design, the optional design with crushed-tuff or quartz sand backfill are analyzed. Thermal-hydrologic calculations are not needed to evaluate the other design options (that is, drip shields and ceramic coatings). The TH results of different design options are shown in Section 3.6.3. Specific repository design data implemented in the TH models of different scale are the following.

3.5.3.1.1 Drift-Scale Repository Design Description

Three-dimensional drift-scale models (for example, the DDT model in the TH multiscale modeling and abstraction method) require heat-decay information for specific waste packages containing different fuel assembly types. Models of this type include the grid refinement necessary for including a number of individual waste packages. It implements a discrete representation (described below) of individual (different) waste packages to be placed in the repository and specifically arranged in the modeled emplacement drift. This includes various-age commercial fuels from PWR as well as BWR.

The CSNF waste-package types are 21 PWR, 12 PWR, 44 BWR, and 24 BWR. The preceding number identifier indicates the quantity of fuel assemblies occurring within a waste package. As an example, a 12 PWR waste package contains twelve fuel assemblies in a single waste package. The individual heat outputs vary from assembly to assembly. From knowledge of the heat output

of each assembly, an average heat decay curve (in Watts/assembly) can be associated with the total number of assemblies making up a specific type. Using as an example the fuel assemblies making up a 12 PWR waste package will illustrate this point. If *X* quantity of assemblies are determined to be appropriate for a particular waste-package type, in this case the 12 PWR waste-package, the average heat of decay curve for *X* assemblies is computed from the knowledge of the individual decay characteristics of each fuel assembly (1, 2, ... , *X*) designated for this waste package type. Knowledge of the total number of assemblies, *X*, along with the capacity of the waste package (in this case 12), fixes the total number of waste packages of this type. Each of the resulting waste packages of a given type has associated with it an average heat output. Using our example, for a 12 PWR waste package and the associated average assembly heat of decay, 12 (assemblies) times 873 (Watts/assembly) equals 10.48 kW. This is an average heat output for a specific 12 PWR waste package to be emplaced in the repository. As an example, there are 155 12 PWR waste packages of this type in the repository.

Each waste package type (12 PWR, 21 PWR, 44 BWR) has an associated average heat output and rate-of-thermal-decay curve. The heat output and rate-of-thermal-decay characteristics are associated with fuel age, burn-up, enrichment, and assembly type as described in waste stream "Case 1" (CRWMS M&O 1997b, Attachment XXXIX). Table 3-22 indicates the initial power output for each of the waste-package types considered in the TSPA-VA TH analyses at the scale of the drift. The heat-of-decay curves implemented for the commercial waste-packages are documented in DTN SNT05071897001.004 (not qualified). As an example of waste package variability in a TSPA-VA model, consider three different 21 PWR waste packages placed in the drift-scale models used in the TH analyses. Three 21 PWR waste packages represent nearly the same percentage to the drift-scale model as the actual number of 21 PWRs (for example, 4,239) would be to the entire repository. Each waste package type makes up a specific (known) percentage of the total repository (obtained from the CDA 1997, pp. 3-15) waste package placement. The idealized number of waste package types represented in the drift-scale model is based on this actual repository percentage. The approach followed in developing a three-dimensional drift-scale model is described in this and the next section, 3.5.3.2.

The quantity of commercial waste packages emplaced in the repository is governed by the total mass of commercial waste to be disposed of and the capacity of individual waste packages. The total mass of commercial waste in the repository is 63,000 MTU (CRWMS M&O 1997e). The commercial fuel waste packages represent 75% of the total waste packages to be emplaced in the repository.

In addition to the commercial waste, individual heat decay data are required for the co-disposal and direct disposal waste packages. These are the additional wastes to be disposed of in the geologic repository at Yucca Mountain. Each co-disposal waste package contains five defense HLW glass logs and one canister of DOE SNF while the direct-disposal waste package contains varying numbers (typically four) of the separate-disposal DOE SNF canisters.

It is assumed that the heat output of each of the co-disposal waste packages is based on a blended average of the total HLW contained in the repository. The heat output of a single DOE SNF canister in the co-disposal waste package is assumed to be negligible when compared to the heat output of the five blended HLW glass logs contained in this package type. The initial heat output of the co-disposal waste package containing five blended HLW glass logs is approximately

4 kW. It is assumed that no aging of the HLW glass occurs before repository emplacement (CRWMS M&O 1997b, pp. 71). The blended average heat output is with respect to the relative amount of Hanford, Savannah River, and West Valley HLW emplaced in the repository. The INEEL HLW glass waste is similar to the West Valley waste and is not considered individually (CRWMS M&O 1997b, pp. 54). The details concerning the additional wastes, both heat output and rate-of-decay, are given in DTN SNT05071897001.004 (the data are not qualified).

The direct-disposal waste package contains four canisters of the N-Reactor fuel component. Since this fuel component makes up nearly 90% of the separate-disposal DOE SNF waste to be emplaced, its heat component is the only DOE SNF waste classification directly considered in the drift-scale analyses for the TSPA-VA. The heat outputs of all other separate-disposal DOE SNF fuels are neglected. It is noted that the heat output of the Navy DOE SNF is indirectly accounted for by an overestimation of the 44 BWR waste-package allotment in the emplacement drift segment applied in the drift-scale models for the TSPA-VA (see Table 3-23). The 44 BWR allotment in the ideal drift segment overestimates the actual allotment of this type by nearly 1%. It is assumed that the overestimate in heat output of the 44 BWR allotment approximates the heat output of the DOE SNF Navy spent fuel.

The N-Reactor fuel will be almost entirely disposed of in the separate (direct-) disposal waste packages. These are the waste packages included in the drift-scale models. Other direct-disposal waste packages are assumed to have negligible heat outputs and are not included in the thermal analyses. The initial heat output of the direct-disposal waste package containing four canisters of N-Reactor fuel is approximately 0.8 kW. Compared to the other waste packages in the model, it is a cold waste package.

The quantity of additional waste packages emplaced in the repository is governed by the total mass of additional waste to be disposed of and the capacity of the specified waste packages. The total mass of additional wastes in the repository is approximately 7,000 MTU (CRWMS M&O 1997e, p. 3-14). The additional waste containers make up about 25% of the total waste packages in the repository.

Waste package representation in the modeled drifts is idealized and based on an approximation of the actual distribution of waste packages of a particular type in the repository. Consequently, this constrains the number of 12 PWR, 21 PWR, 44 BWR, and additional waste packages that can be placed into an idealized drift segment used in a drift-scale model (such as the DDT model in the TH multiscale modeling and abstraction method). Selection of waste package for an idealized drift is also constrained by an overall heat balance with respect to the average characteristics of the repository-wide thermal load at the time of closure. That is, the sequence of waste packages placed in the drift segment nearly reproduce the initial thermal load (in kW/acre) computed for the overall repository (see Section 3.5.3.4 for comparison between the idealized drift and the actual repository-wide thermal load). Differences in the initial thermal load between the idealized drift segment and the average repository output may occur for several reasons. The first is due to approximate waste-package allotments in the drift-scale models. In this case, a limited number of waste packages are not a complete and accurate representation of over 10,200 waste packages in the repository (refer to Table 3-23); it is an approximation driven by computational limitations. The second is a result of heat transfer mechanisms that effectively spread energy along the end lengths of the emplacement drifts. In this case, repository-scale

initial thermal loads are effectively spread over a larger repository area thus reducing the repository thermal loading (in kW/acre). The details of individual waste-package emplacement into an idealized drift segment are discussed in the next section.

3.5.3.2 Emplacement Drift Geometry and Waste Package Layout Information for Drift-Scale Models

It is assumed that the thermal decay curves for a limited number of waste package types are representative of a wide range of waste packages to be emplaced in the repository as described in the following. The selected waste-package types span the range of heat output, from the high-output CSNF waste packages to the low-output direct-disposal waste package containing the DOE SNF canisters. The drift-scale models used in TSPA-VA contain a total of seven waste packages along the length of a modeled emplacement drift (see Figure 3-39) for the reference point load repository design. Five and one-half are CSNF waste packages. The remaining one and one-half waste packages are co-disposal including the defense HLW and direct-disposal including a single component of the separate-disposal DOE SNF.

Three types of CSNF (12 PWR, 21 PWR, 44 BWR) as well as the representative additional wastes have their expected inventory (e.g., number of waste packages) and relative inventory percentages shown in Table 3-23. This table indicates how a representative section of the repository can be modeled with as few as seven waste packages. The discrete drift section represents the allotment of different package types by reducing the total numbers of each type considered while maintaining the relative proportions emplaced in the repository. The total number of waste packages emplaced in the repository is obtained from CRWMS M&O (1997e, pp.3-15). The approximation of seven waste packages in the idealized drift nearly approaches the actual representation of the repository waste stream (for example, 5.4% of the expected repository inventory is 12 PWR, while the idealized drift contains 7.1% by inventory of the 12 PWR). It is also noted that a single waste package type is neglected from the idealized representation entirely. That is, the relatively small contribution of the 24 BWR waste packages (49 total) in the repository has been neglected in the drift-scale model. The idealized drift segment is made exact if, and only if, the modeled number of waste packages is identical to the actual number of waste packages.

The idealized drift segment used in the TSPA-VA base case TH contains CSNF waste packages including three 21 PWR, two 44 BWR, and one-half 12 PWR waste packages. One of the CSNF waste packages included in the model is a 21 PWR design-basis fuel. It is somewhat hotter than the average 21 PWR waste package upon receipt into the repository and represents a potential maximum initial heat output at the time of emplacement (approximately 18 kW). This package is thermally balanced with a cooler (approximately 3 kW) 21 PWR waste package. This provides a balanced initial heat load when compared to the repository thermal load. It results in an averaged emplacement drift heat load. As a sensitivity study, two different emplacement drift segments are considered in Section 3.6.4 of this chapter. The base-case segment described in this section is compared to a "cold" drift segment containing lower heat output waste packages and to a "hot" drift segment containing higher heat output waste packages. As indicated above, the additional wastes do not occupy their own space in the geologic repository; they are placed between the commercial waste packages as described above.

In order to maintain a 1.0-meter minimum spacing between all waste packages (CRWMS M&O 1997d, pp. 14), the co-disposal waste package is placed between the design-basis 21 PWR and an "average" heat output 21 PWR. The direct-disposal waste package is placed at the end of the drift segment next to the 44 BWR waste packages. Refer to Figure 3-39 for the exact locations of each waste package type. This figure also indicates the mass loading of each commercial container (CRWMS M&O 1997e, pp. 3-17) with the associated initial heat outputs (in kW) for each of the waste package types implemented in the base-case drift segment. Physical characteristics of the waste package are also indicated in this figure. Emplacement drift design/geometry as well as waste-package emplacement and physical characteristics are based on data obtained by PA from subsurface design as well as waste-package-design following the abstraction/testing workshops in CRWMS M&O (1997c); CRWMS M&O 1997d; and QAP 3-12 (MOL.19980720.045). The data obtained from CRWMS M&O (1997c), are unqualified.

The point loaded repository AML is 85 MTU/acre, with a specified 28-meter drift spacing. This specifies the mode of waste package placement in the repository. The above information along with mass content constrains the waste package spacing in the drift. Reference to Figure 3-39 indicates that the average waste package spacing is on the order of one-half drift spacing. This is a feature of the point-loaded repository. The specific waste package spacing is computed for each type based on the following:

$$AML = 4046.86\ \Sigma MTU/S_{wp}S_d \qquad (3\text{-}17)$$

where 4046.86 is a conversion factor between square meters and acres, ΣMTU is the sum of container mass (in MTU), and S_{wp} and S_d are the waste package and drift spacing in meters, respectively. As an example, take the average 21 PWR shown in Figure 3-39. Given an AML of 85 MTU/acre, a drift spacing of 28-meters, and a waste-package capacity of 8.93 MTU, the spacing for this waste-package is:

$$Swp = [(4046.86)\ (8.93)]/[(85)(28)] = 15.18 \text{ meter} \qquad (3\text{-}18)$$

Since the spacing between some CSNF waste packages is large enough, emplacement of additional waste packages between CSNF packages can result without an increase in the potential repository area. Therefore, the reference AML of 85 MTU/acre is based on the commercial waste only. It is reiterated that the heat output of all waste packages (commercial and additional) is included in the total heat output of this point-load drift segment.

3.5.3.2.1 Emplacement-Drift Geometry

The modeled emplacement-drift geometry for TH analyses is based on recent work from the subsurface design organization (see also CRWMS M&O 1997c, pp. 57 and 58; and CRWMS M&O 1997d, pp. 14). The information obtained from the subsurface design organization included details regarding the inside diameter of the drift, the thickness of the concrete liner, and the height of the invert material (specified in the current analysis as a concrete invert).

The details of the emplacement-drift geometry are given in Table 3-24. In order to facilitate the use of the rectangular XYZ mesh generator in the NUFT code (Nitao 1996), the actual cylindrical drift is transformed into an equivalent volume (and therefore cross-sectional area)

XYZ cross-sectional model. It is cross-sectional equivalent square drift geometry (refer to Table 3-25). This assumption has been implemented in order to maintain consistency with the ongoing drift-scale models being developed by the LLNL near-field TH modeling tasks (Buscheck 1996; Hardin 1998, Chapter 3). This has been found in previous studies to be an adequate assumption (Hardin 1998, pp 3-35) based on a comparison of waste package temperature and the temperature difference between waste package and drift wall for circular and for cross-sectional area equivalent square geometrics (Busheck 1996, p. 1.10-23).

The modeled geometry is given in Table 3-25. It is required that the volume fraction of invert inside the drift in the modeled geometry be identical to that of an actual emplacement drift. Therefore, the following equation is applied to compute the height of the invert in the drift-scale model:

$$h_{inv} = \frac{4A_{inv}h_{id}}{\pi d_{id}^2} \tag{3-19}$$

where A_{inv} is the actual cross-sectional area of the invert, h_{id} is the model width (and height) of the drift, h_{inv} is the modeled height of the invert material, and d_{id} is the inner diameter of the emplacement drift.

3.5.3.2.2 Waste Package Geometry

Diameters and lengths of the waste packages are given in Table 3-26 (actual values obtained according to the QAP3-12 (MOL.19980720.045), design input transmittal process, dated 9/10/97). The physical dimensions of the waste packages listed in Table 3-26 are unqualified. The table includes the actual value along with the modeled value. The modeled values are volume-equivalent quantities for and average waste package diameter in a rectangular coordinate system in order to make use of the mesh generator in the NUFT flow code. Also, the additional waste package diameters are set equal to the CSNF waste-package diameters in order to reduce the gridding complexity within the modeled emplacement drift (i.e., to reduce the level of complexity when computing the required view factors, etc.). This is assumed to be reasonable since the actual waste-package dimensions listed for the additional waste packages are given as "not to exceed" dimensions. The outer diameter of the waste package applied to each of the modeled waste packages is based on an average 1.63-meter diameter obtained from the actual waste-package data given in Table 3-26.

3.5.3.3 Mountain-Scale Design Description

The mountain-scale TH models require an average thermal-load representative of all wastes emplaced at Yucca Mountain. The repository-wide thermal load can be characterized by a uniform radioactive heat-of-decay curve, which is a blended average of the heat-of-decay curves from the entire inventory of waste packages emplaced in the repository. Models of this type implement a smeared-heat source based on blended average fuel characteristics. As a result, the total repository-wide thermal load includes contributions from the all PWR and BWR assemblies (CRWMS M&O 1997b), the total HLW glass assemblies, and the separate-disposal DOE SNF

(N-Reactor fuel) expected to be placed into the repository. The thermal loading data required for the TSPA-VA analyses are documented in detail in DTN: SNT05071897001.004. The thermal loading data developed for the viability assessment thermal and thermal-hydrologic calculations are unqualified data. The following sections detail the repository design requirements necessary for the mountain-scale models.

3.5.3.3.1 Calculation of the Repository Area

The areal extent of the geologic repository (or repository footprint) is based on the AML for the reference design. For an 85 MTU/acre repository with 63,000 MTU of commercial waste (CRWMS M&O 1997d, pp. 3 of 55 and 23 of 55), the repository plan area, A_{rep}, is:

$$\text{Arep} = 63{,}000 \text{ MTU} / 85 \text{ MTU/acre} = 741.2 \text{ acre} \tag{3-20}$$

This area is identical to the value reported in (CRWMS M&O 1997f, pp.15). There is additional area left unloaded and designated as a contingency area. This corresponds to 15 empty emplacement drifts at the southern end of the repository. Additionally, about 32 meters of unloaded drift length exist at either end of an emplacement drift. For the base case, the AML of 85 MTU/acre includes only the mass of commercial waste. The additional wastes (direct-disposal or co-disposal waste packages) are placed between commercial-waste packages so that no additional area is required in the repository. The heat output of the additional waste is included in the drift-scale model formulations as well as in the repository-wide thermal load for the mountain-scale models.

3.5.3.3.2 Calculation of the Total Repository Thermal Load

The initial thermal load, TL, of the repository is computed as follows:

$$TL = \frac{Q}{A_{rep}} \qquad (kW/acre) \tag{3-21}$$

where Q is the blended heat output of all repository wastes at the time of waste emplacement (t = 0). It is assumed for the base-case analyses that the waste is simultaneously emplaced in the year 2010 and that no aging occurs at the time of initial emplacement. In order to determine the appropriateness of this assumption, a sensitivity study using a delayed thermal load of 10, 20, 50, and 100 years is considered at the scale of the mountain. An example of an initial thermal load with a 10-year delay is computed with Q (at t = 10 years) instead of Q (at t = 0 years) based on Figure 8-41. For this thermal delay example, the initial thermal load is approximately 78 kW/acre. The results of this study are shown in Section 3.6.4.3. For the base case, the initial thermal load is obtained for simultaneous emplacement as follows (CRWMS M&O 1997b, Attachment XXZII, pp. 1 and 2; CRWMS M&O 1997e; personal communication with Chris Stockman and Ron McCurly, INEEL modeling information and heat decay data for the N-Reactor fuel data, September 1997 [LEE]).

$$TL = \frac{73{,}670 \quad kW}{741.2 acre} \approx 99. \frac{kW}{acre} \tag{3-22}$$

where the total Q (= 73,670 kW) contains the heat output from 8,314 canisters of HLW glass, 433 canisters of separate-disposal DOE SNF N-Reactor fuel, 94,847 PWR assemblies, and 124,269 BWR assemblies. The total heat output is based on the averaged characteristics of each fuel type (e.g., PWR or BWR) multiplied by the total number of assemblies. It is assumed in Equation (3-22) that the HLW glass is emplaced without aging (CRWMS M&O 1997b, p. 71 of 75). It is also assumed that the total heat output of the other forms of separate-disposal DOE SNF is small in comparison to the total heat output associated with the N-Reactor fuel component. This is assumed reasonable since the N-Reactor fuel makes up approximately 90% of the 2,333 MTU of separate-disposal DOE SNF emplaced in the repository.

The result given in Equation (3-22) is a function of the waste stream characteristics of the assemblies designated for emplacement. Waste stream "Case 1" in (CRWMS M&O, 1997b, pp. 40 and 41 of 75, Attachment XXXIX) is used for reference repository design heat output and thermal decay over time. Different waste streams will result in different initial thermal loads (true for simultaneous emplacement in either case). Additionally, the resultant initial thermal load at the scale of the mountain may vary slightly from the value given in Equation (3-22) as a result of heat transfer mechanisms that effectively spread heat along the empty ends of the drift, thereby increasing the emplaced area. The thermal rate-of-decay curve for the repository-wide thermal load is shown in Figure 3-41.

3.5.3.4 Heat Loading Information

As previously discussed, the geometry of the emplacement drift segment, as shown in Figure 3-39, results in an AML of 85 MTU/acre. Since the AML does not capture the variability in the rate of heat release from a waste package, the areal power density of the system must also be considered when selecting waste packages for inclusion in the drift-scale models.

The initial areal power density (APD) in the seven-waste-package drift-scale models, with the additional waste included, is approximately 99.9 kW/acre. The initial APD of the CSNF waste packages in the idealized drift model is about 91.4 kW/acre. The initial APD for all commercial-waste packages in the actual repository is approximately 91.3 kW/acre, with the total, including the additional waste, about 100.6 kW/acre. The slight difference in CNSF APD is due to the discrete nature of the drift-scale model used to represent the repository totals of each waste-package type. Additionally, the discrete nature of the drift model causes the total APD to differ slightly from Equation (3-22) due to the discrete nature of the drift model and the inexact representation of the additional wastes (25% actual vs. 21.4% modeled). Finally, partial filling of late-entry waste packages is not included in the drift models but is included in the mountain-scale models by using the actual total assemblies emplaced in the repository. As an example, a 21 PWR waste package in the idealized drift-scale model contains exactly 21 assemblies. In actuality, a limited number of 21 PWR waste packages may contain fewer than the total 21 assemblies due to filling procedures during repository loading period. This cannot be accounted for in our idealized drift segment. Unlike the AML (which is constant in time), the APD varies with time as the heat output decays in time based on the heat-of-decay data for each of the fuel types. Table 3-27 contains vital thermal loading data (initial) applied in drift- and mountain-scale models.

This lineal power load of the commercial fuel only (0.63 kW/m in Table 3-27) is compared to the value used in CRWMS M&O 1997d, Attachment IV, p. 39) as 0.62 kW/m. The thermal loads are nearly identical. The small difference is because of the waste package variability accounted for in the TSPA TH models. It is necessary for TSPA to include waste package variability within the TH models in order to accommodate the waste package corrosion rate models component of TSPA-VA. The drift segment designed by performance assessments (see Figure 3-39) contains waste-package variability while still maintaining the average repository-wide thermal loading characteristics. The drift segment contained in CRWMS M&O (1997d, p. 39) is for average characteristics of each waste-package type, 12 PWR, 21 PWR, and 44 BWR. It also maintains the average repository-wide thermal loading characteristics. It is emphasized that the comparison given above is for the commercial fuel only. A comparison cannot be made for the total lineal power load (which includes CSNF, HLW, and separate-disposal DOE SNF in the TSPA thermal models) since the drift segment given in CRWMS M&O (1997d, p. 39) is for a previous repository design containing a four-pack HLW package for a total 7,000 MTU of HLW. Recall that the TSPA models apply a five-pack HLW package for 4,667 MTU and a four-pack direct-disposal waste package for 2,333 MTU of separate-disposal DOE SNF. However, since this does not influence spacing of waste packages (recall that the additional wastes do not occupy their own space in the repository), the comparison of the CSNF values is still valid for these two drift-segment models.

3.5.4 TH Analyses

3.5.4.1 Mountain-Scale Analyses

Thermally Perturbed Liquid-Phase Flow Below the Repository Horizon - The heating of the rocks near the repository will alter the liquid-phase flow field in the UZ. Below the repository, the water flux will change as the repository heats up and then cools down. As the repository heats up, water is initially driven away from the heat source as a dryout zone develops around the repository. The heated dryout zone can prevent the infiltrating water from moving down through the repository resulting in a drop in the water flux at repository depth. Next, the heat output from the repository will drop until it is not sufficient to maintain a steam zone, and the water that had accumulated above the steam zone will drain through the repository horizon to the water table. Eventually, the heat output is small enough not to affect the liquid flow field so that it returns to a steady state.

The duration of the temporal change in the water flow field resulting from the thermal perturbation can become an important parameter in determining the rate of transport of radionuclides through the UZ and to the water table. Clearly, if the duration and the change in magnitude of the water flow field perturbation are not large, then the transport of radionuclides can be analyzed only by considering the steady-state UZ flow fields (Ho et al. 1996, Ho et al. 1997, Ho 1997). In Chapter 5 of the TSPA-VA Technical Basis Document, less than 1% of the total waste packages have failed by a corrosion mechanism 10,000 years after waste emplacement. Consequently, perturbations in the UZ flow fields during the first 5,000 years after waste emplacement in Yucca Mountain were assumed to be negligible. It should be noted here that juvenile failures (presumably occurring in the first 100 years or so) were assumed to be small in number. The unsaturated zone flow fields used did not include any permanent alteration due to coupled thermal-hydrologic-chemical-mechanical effects.

The vertical liquid flux through model elements below the elements that represented the "center" and "edge" of the repository were extracted from two-dimensional TH mountain-scale simulations. The cross-section (refer to Figure 3-3) was located at northing = 233,400m with the "center" located at easting = 170,650m and the "edge" located at the eastern edge of the repository at easting = 171,200m (refer to Figure 3-3). The base-case rock properties were used (DTN LB971212001254.001, LB971212001254.002, LB971212001254.003, LB971212001254.004, and LB971212001254.005; these hydrologic data are not qualified). The five base case rock property sets contain variability in infiltration rates and in the fracture van Genuchten α_f parameter. One base-case set is calibrated for the nominal present-day infiltration rate and a mean van Genuchten α_f. The other four base-case parameter sets are calibrated at a combination of a third or three times the present-day infiltration rate and higher and lower values of the van Genuchten α_f parameter. A total of ten base-case simulations were performed with each of the five property sets being run at present-day and at climate-change (long-term-average) infiltration boundary conditions.

The liquid fluxes for three different cases are presented in Figures 3-42 through 3-47 at different locations below the repository horizon and above the water table. They represent the base-case α_f mean, nominal I infiltration, the base-case α_f maximum, I/3 infiltration, and the base-case α_f maximum I*3 LTA infiltration. The average infiltration rates *over the cross Section* for the three cases are 7.96 mm/year (DTN GS960908312211.003, these data are qualified), 2.65 mm/year (DTN GS960908312211.003, these data are qualified), and 136 mm/year respectively. The repository-wide heat decay power curve (DTN SNT05071897001.004, these data are not qualified) used in the simulations can be found in Figure 3-41. The nomenclature of the layers in the figures is as follows: TSw35 (Topopah Springs welded 5), TSw36 (Topopah Springs welded 6), CH1vc (Calico Hills vitric 1), CH2vc (Calico Hills vitric 2), CH3zc (Calico Hills zeolitic 3), CH4zc (Calico Hills zeolitic 4), PP3vp (Prow Pass vitric 3), PP2zp (Prow Pass zeolitic 2), and the BF3vb (Bull Frog vitric 3).

Figure 3-42 shows the vertical liquid flow for the base-case nominal I infiltration in several geologic units below the center of the repository. The ambient liquid flux through the layers below the repository is 4×10^{-7} kg/m^{2}s. The liquid flux increased by a factor of 12 to 5.3 $\times 10^{-6}$ kg/m^{2}s ten years after waste emplacement in the TSw35 unit and then slowly returned to the ambient value after 5,000 years. In the TSw36 unit, 93 meters below the repository, the liquid-water flux increased by a factor of four after twenty years and returned to the steady-state value after 2,000 years. In the Calico Hills, Prow Pass, and Bullfrog units, the increase in liquid flux decreased in magnitude as the distance from the repository increased. The liquid flux in these locations all returned to within a factor of two of the ambient flux after only 200 years and reached ambient values after 2,000 years.

At the edges of the repository (Figure 3-43), the infiltration rates are much lower, so the local steady-state liquid fluxes at the edge of the repository are also lower. The peak liquid flux through the repository TSw35 unit was 4.5×10^{-6} kg/m^{2}s ten years after waste emplacement. The liquid flux returned to the steady-state value after 2,000 years. The liquid flux in the geologic units below the repository fluctuated between 10 and 1,000 years but the fractional increase was much smaller than was seen at TSw35 host unit. The liquid flux in those elements also returned to the steady-state value after 2,000 years.

The vertical liquid fluxes from the base-case α-maximum, I/3 infiltration rate simulation are presented in Figures 3-44 and 3-45. The lower infiltration rate results in lower steady-state liquid flow rates through the mountain. Near the center of the repository, the peak flux takes place at the same time as it did in the base-case simulation. The liquid flux in the regions below the repository peak, as the region of dryout grows and then decreases as the repository above, begin to re-wet. After 5,000 years, the locations below the repository have all returned to steady-state but it takes an additional 2,000 years for the repository to return to the steady state water-flux value.

The vertical liquid fluxes at the edge of the repository for the base-case α-maximum, I/3 infiltration rate simulation (Figure 3-45) look very similar to that for the base-case infiltration. All of the liquid fluxes returned to the ambient values after 2,000 years.

The vertical liquid fluxes for the base-case α-maximum, I*3 long-term-average infiltration rate are presented in Figures 3-46 and 3-47. The high ambient infiltration rate results in high liquid-flow rates in all layers shown in the figures. At the center of the repository, the liquid flux in the TSw35 increased by a factor of two at 15 years and returned to ambient values after 2,000 years. In all of the lower units, the liquid flux did not increase by more than 10% during the duration of the simulations. At the edge, similar trends in liquid flux were seen.

From the results of the cases spanning infiltration rates (over the cross-section) of 2.65 mm/year to 136 mm/year, it was concluded that the potential alteration of the thermal perturbation on liquid-phase fluxes below the repository horizon was short lived. Water fluxes below the repository horizon, the region where radionuclide transport occurs, returned to ambient in 5,000 years or less. The simulations for which the liquid fluxes were perturbed the longest were the low-infiltration-rate cases. For higher infiltration rates, the thermal perturbation lasted 2,000 years or less. Therefore, for waste package breaches after the first 1,000 years, radionuclide transport calculations performed in RIP can be based on ambient flow fields alone. This assumption neglects permanent changes due to dissolution and precipitation of minerals.

3.5.4.2 Drift-Scale Analyses

3.5.4.2.1 Procedure for Calculating Engineered-Barrier System Thermal Hydrologic Conditions

Complementary one-dimensional SDT submodels, two-dimensional LDTH submodels, and three-dimensional DDT submodels (Figure 3-30a ,b, and c) are calculated for locations that are regularly spaced throughout the repository area, as described previously. The calculation procedure used to obtain the drift thermodynamic environment is described in detail in the following.

Briefly, for each location, parallel SDT and LDTH calculations are conducted for AMLs of 85, 56.67, and 42.5 MTU/acre (the lower two values represent cooler areas in the repository such as repository edges). This results in 6 model calculations (three for SDT and three for LDTH) per location or 210 calculations for the 5×7 grid.

In addition, one DDT submodel calculation is required by the TH multiscale modeling and abstraction method.

This procedure captures the significant effects from mountain-scale heat flow as well as drift-scale TH behavior driven by heat output from individual waste packages, each having distinctively different heat generation characteristics. To explicitly account for these effects in a single numerical TH model would require approximately 60 million grid blocks, which is beyond the computational capabilities of the current generation of TH simulators.

Altogether, using the 5×7 grid, a single TSPA-VA TH scenario requires 424 NUFT runs, including 210 one- and two-dimensional drift-scale calculations, one three-dimensional drift-scale calculation, and one mountain-scale calculation. In a procedure that conditions the comparison of thermal conduction and TH model calculations, an additional 212 runs are used to initialize the models. Using the NUFT code, which is optimized for efficiency, a complete set of 424 runs requires 12 to 16 hr on 9 Sun Ultra2 Sparc workstation processors.

The TH multiscale modeling and abstraction method (described in Section 3.5.1) can be used to evaluate alternative TH parameter sets, such as the following:

- Preliminary base-case property set
- Base-case property set
- "Thermal-Hydrologic Property Set"
- Dual permeability/Weeps property set.

The TH multiscale modeling and abstraction method is also repeated to evaluate alternative repository models, including the reference point-load design, the line-load designs, and the use of engineered backfill in emplacement drifts.

The TH multiscale modeling and abstraction method is outlined in Figures 3-48 and 3-49. The intermediate results of the calculation procedure are shown as the orange boxes in Figures 3-48 and 3-49. The interpolation/calculation steps are shown as the green boxes. This procedure involves seven major calculation steps, with several of the steps consisting of multiple parts. The calculational steps for cases with engineered backfill (Figure 3-49) are slightly different from those of cases with no engineered backfill (Figure 3-48). Note that the calculational procedure for cases with engineered backfill has been revised relative to that described in the Near-Field/Altered Zone Models Report (Hardin 1998).

Step 1—Conduct Numerical Simulations Using NUFT

The first step is to conduct numerical-model calculations with the use of the NUFT code (shown as blue boxes in Figures 3-48 and 3-49), including the following submodels:

- SMT model (1 model run)
- SDT model (105 model runs)
- LDTH model using DKM (105 model runs)
- DDT model (1 model run)

Step 2—Construct Scanning Curves

The second step is to construct the functional relations, called scanning curves, among the various model-output variables from complementary drift-scale models (shown as yellow boxes in Figure 3-48 and 3-49). The scanning curves include the following:

- Drift-wall TH temperature vs. drift-scale, smeared-heat source, conduction-only temperature

  T_{dw}(LDTH) vs. T_{rep}(SDT), which is the LDTH-predicted drift-wall temperature T_{dw} vs. the SDT-predicted host-rock temperature T_{rep} (Figure 3-50a). This requires the parallel use of the LDTH and of SDT models. The variable T_{dw} is the average over the perimeter of the drift wall. This relation is developed for all 35 locations, with AMLs of 85, 56.67, and 42.5 MTU/acre. The three different AML "scanning" curves in Figure 3-50a guide the interpolation (in Step 3) of the local scanning curve that reflects the influence of local heating conditions and percolation flux on T_{dw} in a given region of the repository. At the center of the repository, it is likely that the 85-MTU/acre curve will apply; close to the repository edge, cooling may cause the local scanning curve to lie closer to the lower AML curves.

- Drift-wall TH relative humidity vs. drift-wall TH temperature

  RH_{dw}(LDTH) vs. T_{dw}(LDTH), which is the LDTH-predicted, drift-wall relative humidity RH_{dw} vs. drift-wall temperature T_{dw} (Figure 3-50b). The variables T_{dw} and RH_{dw} are averages over the perimeter of the drift wall. This relation is developed for all 35 locations and AMLs of 85, 56.67, and 42.5 MTU/acre. The three different AML scanning curves in Figure 3-50b guide the interpolation (in Step 5) of the local scanning curve that reflects the influence of local heating conditions and percolation flux on dryout behavior at a given location in the repository. During the heat-up phase, nonequilibrium fracture–matrix behavior causes a lag in rock dryout (and reduction in relative humidity), making it necessary for T_{dw} to rise well above the nominal boiling point before dryout begins. During cool-down, rewetting (and relative humidity rise) lags behind the decline in T_{dw}.

- Backfill TH RH_{ratio} vs. backfill TH temperature difference

  RH_{ratio}(LDTH) vs. ΔT_{bf}(LDTH), where RH_{ratio}(LDTH) = RH_{bf}(LDTH)/RH_{dw}(LDTH) and ΔT_{bf}(LDTH) = T_{bf}(LDTH) -T_{dw}(LDTH), where RH_{bf} and T_{bf} are the LDTH-predicted, backfill relative humidity and temperature, respectively, averaged over the perimeter of the waste package, and RH_{dw} and T_{dw} are the LDTH-predicted, drift-wall relative humidity and temperature, respectively, averaged over the perimeter of the drift wall (Figure 3-50g). The variable RH_{bf} is determined for the backfill gridblocks adjacent to the waste package. The relation RH_{ratio}(LDTH) vs. ΔT_{bf}(LDTH) is developed for all 35 locations and AMLs of 85, 56.67, and 42.5 MTU/acre. The three different AML scanning curves in Figure 3-50g guide the interpolation (in Step 7) of the local scanning curve that reflects the influence of seepage into the drift and

capillary-driven wicking of moisture in the backfill at a given location in the repository. This substep, which applies only to cases with engineered backfill, provides input for Step 7.

- Drift-wall TH matrix saturation vs. drift-wall TH temperature

  S_{liq}(LDTH) vs. T_{dw}(LDTH), which is the LDTH-predicted, drift-wall liquid-phase saturation S_{liq} vs. drift-wall temperature T_{dw} (Figure 3-50c) The variables T_{dw} and S_{liq} are averages over the perimeter of the drift wall. This relation is developed for all 35 locations and AMLs of 85, 56.67, and 42.5 MTU/acre. The three different AML scanning curves in Figure 3-50c guide the interpolation (in Step 5) of the local scanning curve that reflects the local heating conditions and dryout conditions at a given location in the repository. During the heat-up phase, nonequilibrium fracture–matrix behavior causes a lag in rock dryout (and S_{liq} reduction), making it necessary for T_{dw} to rise well above the nominal boiling point before dryout begins. During cool-down, rewetting (and S_{liq} rise) lags behind the decline in T_{dw}.

- Invert TH liquid saturation vs. lower drift-wall TH temperature

  $S_{liq,inv}$(LDTH) vs. T_{ldw}(LDTH), which is the LDTH-model-predicted liquid-phase saturation in the invert vs. the temperature T_{ldw} at the lower drift wall (Figure 3-50f). This relation is developed for AMLs of 85, 56.67, and 42.5 MTU/acre and the l4c3 drift-scale model location (Table 3-11). The three different AML scanning curves in Figure 3-50f guide the interpolation (in Step 5) of the local scanning curve that reflects the influence of local heating conditions on dryout behavior in the invert at a given location in the repository.

- Drift-wall conduction-only axial temperature variation

  ΔT_{dw}(DDT; waste-package type), which is the DDT-predicted temperature deviation ΔT_{dw} from the average drift-wall temperature, axially along the drift, for a given waste package type (Figure 3-51a). This step is required to modify the LDTH-predicted T_{dw} to account for the influence of local heating conditions produced by the waste-package emplacement sequence (see Step 4). The value of ΔT_{dw} will generally be positive for the point-load design because of the large gaps (in the axial direction) between waste packages. Locations of hot-waste packages will have a large positive ΔT_{dw}, particularly at early time; locations of cool-waste packages will have a negative ΔT_{dw}. The value ΔT_{dw} is determined for each waste-package location in the DDT model by subtracting the average T_{dw} along the entire drift in the DDT model from the local T_{dw} at a given waste-package location. This relation is developed for an AML of 85 MTU/acre and the l4c3 drift-scale model location, which is at the geographic center of the repository layout.

- Waste-package conduction-only axial temperature variation

  ΔT_{wp}(DDT; waste package-type), which is the DDT-predicted temperature difference ΔT_{wp} between the waste package and drift wall for a given waste-package type (Figure 3-51b). This calculation is required in order to predict the temperature of the waste package. The value of ΔT_{wp} will always be positive for all waste-package locations except for the colder direct-disposal waste package since the local temperature for this waste package is less than the drift-length averaged temperature obtained from the DDT model. Locations of hot-waste packages will have a large ΔT_{wp}, particularly at early time; locations of cool-waste packages will have a smaller ΔT_{wp}. For backfill cases, ΔT_{wp} will be extremely large, particularly immediately after backfill is emplaced. The value ΔT_{wp} is determined for each waste-package in the DDT model by subtracting the average T_{dw} along the entire drift in the DDT model from the waste-package temperature T_{wp}. This relation is developed for an AML of 85 MTU/acre and the l4c3 drift-scale model location, which is at the geographic center of the repository layout. This location represents a slightly higher infiltration rate (~11 mm/year) when compared to the average over the entire repository footprint (~8 mm/year).

- Waste-package, conduction-only, local-temperature difference for backfill cases

  $\Delta T_{wp,local}$(DDT; waste-package type) = T_{wp}(DDT; waste-package type) -$T_{dw,local}$(DDT; waste-package type), where T_{wp} is the DDT-predicted waste-package temperature and $T_{dw,local}$ is the DDT-predicted, local, drift-wall temperature for a given waste-package location (Figure 3-51e). The variable $T_{dw,local}$ is averaged over the perimeter of the drift wall at a given waste-package location. The value of $\Delta T_{wp,local}$ will always be positive for all waste-package locations. Hot-waste package locations will have a large $\Delta T_{wp,local}$, particularly immediately after backfill is emplaced; cool-waste package locations will have a smaller $\Delta T_{wp,local}$. The relation for $\Delta T_{wp,local}$(DDT; waste-package type) is developed for an AML of 85 MTU/acre and the l5c2 drift-scale model location, which is close to the geographic center of the repository layout and is more representative (~ 8.5 mm/year) of the average infiltration flux over the repository footprint. This substep, which applies only to cases with engineered backfill, provides input for Step 7.

Step 3—Interpolate the Distribution of Average Drift-Wall Temperature

The drift-wall temperature corresponding to a three-dimensional mountain-scale TH model with emplacement drifts modeled by line-average heat sources is approximated by interpolating scanning curves. The interpolant T_{dw}(LMTH; x,y) is calculated for average drift-wall conditions using the smeared-heat-source repository temperature T_{rep}(SMT; x,y), and the T_{dw}(LDTH) vs. T_{rep}(SDT) scanning curve, at the 35 locations and three AMLs (Figure 3-50a) (Note: x, y indicate different repository locations such as an easting and northing coordinate). This process involves spatial interpolation among the 35 locations and also involves interpolation among the three AML scanning curves in Figure 3-50a. The result of this step is the distribution of average drift-wall temperatures as a function of location in the repository. Because this process

approximates a three-dimensional LMTH-model prediction of the distribution of T_{dw} in the repository, the resulting distribution is called T_{dw}(LMTH; x,y).

Step 4—Interpolate the Distribution of Drift-Wall and Backfill Temperature for Each Waste-Package Type

The drift-wall temperature distribution in the repository, as a function of location, is calculated for each waste-package type by adding ΔT_{dw}(DDT; waste-package type) to the T_{dw}(LMTH; x,y) distribution determined in step 3. The net result of this step is assumed to be comparable to having a three-dimensional DMTH model prediction of the drift wall temperature T_{dw} distribution in the repository for each waste-package type; hence, the resulting distribution is called T_{dw}(DMTH; x,y, waste-package type), where x and y refer to the coordinate location in the repository. The drift wall temperature including hydology and waste package variability at any repository location is:

$$T_{dw}(\text{DMTH}; x, y, \text{waste package} - \text{type}) = T_{dw}(\text{LMTH}; x, y) + \Delta T_{dw}(\text{DDT; waste package - type})$$

or,

a result of Step 4 = the result of Step 3 + a result of Step 2

The backfill temperature distribution in the repository, as a function of location, is calculated for each waste-package type by adding $\Delta T_{wp.local}$(DDT; waste-package type) determined in Step 2 to the T_{dw}(LMTH; x,y) distribution determined in Step 3. The net result of this step is assumed to be comparable to having a three-dimensional DMTH model prediction of the T_{bf} distribution in the repository for each waste-package type; hence, the resulting distribution is called T_{bf}(DMTH; x,y, waste-package type). This substep applies only to cases with engineered backfill. The backfill temperature for each waste package type is computed from:

$$T_{bf}(\text{DMTH}; x, y, \text{waste package} - \text{type}) = T_{dw}(\text{LMTH}; x, y) + \Delta T_{wp,local}(\text{DDT; waste package - type})$$

or,

a result of Step 4 (for backfill only) = the result of Step 3 + a result of Step 2

Step 5—Interpolate the Distribution of Near-Field and In-Drift Hydrologic Conditions

This step involves interpolating the distribution of near-field and in-drift TH conditions in the repository for each waste-package type using the temperature distribution from Step 4 and the scanning curves from Step 2. The relative humidity at the waste package, the drift-wall matrix saturation and the invert liquid-phase saturation are calculated by interpolation for each waste-package type, as a function of location in the repository.

- Relative humidity at the drift wall

  RH_{dw}(DMTH; x,y, waste-package type), which is the distribution of relative humidity for each waste-package type, is interpolated using the abstracted drift-wall temperature T_{dw}(DMTH; x,y, waste package-type) and the drift-wall relative humidity RH_{dw}(LDTH) vs. T_{dw}(LDTH) scanning curve at the 35 locations and three AMLs (Figure 3-50b). This process involves spatial interpolation among the 35 locations and interpolation among the three AML scanning curves in Figure 3-50b. The result of this step is assumed to be comparable to having a DMTH-model prediction of the distribution of RH_{dw} in the repository for each waste-package type; hence, the resulting distribution is called RH_{dw}(DMTH; x,y, waste-package type), where x and y refer to the coordinate location in the repository.

- Drift-wall matrix saturation

  S_{liq}(DMTH; x,y, waste-package type), which is the distribution of saturation for each waste-package type, is interpolated using the abstracted drift-wall temperature T_{dw}(DMTH; x,y, waste package-type) and the drift-wall liquid-phase saturation S_{liq} (LDTH) vs. T_{dw}(LDTH) scanning curve at the 35 locations and three AMLs (Figure 3-50c). This process involves spatial interpolation among the 35 locations and interpolation among the three AML scanning curves in Figure 3-50c. The result of this step is assumed to be comparable to having a DMTH-model prediction of the distribution of S_{liq} in the repository for each waste-package type; hence, the resulting distribution is called S_{liq} (DMTH; x,y, waste-package type), where x and y refer to the coordinate location in the repository.

- Invert liquid-phase saturation

  $S_{liq,inv}$ (DMTH; x,y, waste-package type), which is the invert liquid saturation for each waste-package type, is interpolated using the abstracted drift-wall temperature T_{dw}(DMTH; x,y, waste-package type) and the invert liquid-phase saturation $S_{liq,inv}$ (LDTH) vs. lower drift-wall temperature T_{ldw}(LDTH) scanning curve at the 35 locations and three AMLs (Figure 3-50f). This process involves spatial interpolation among the 35 locations and interpolation among the three AML scanning curves in Figure 3-50f. The result of this step is assumed to be comparable to having a DMTH-model prediction of the distribution of $S_{liq,inv}$ in the repository for each waste-package type; hence, the resulting distribution is called $S_{liq,inv}$ (DMTH; x,y, waste-package type), where x and y refer to the coordinate location in the repository.

Step 6—Determine the Distribution of Waste-Package Temperature for Each Waste Package Type

Step 6 is to use the drift-wall temperature distribution from Step 3 and scanning curves from Step 2 to determine the distribution of temperature on waste packages throughout the repository area for each waste-package type. The result is the abstracted waste-package temperature distribution (T_{wp}) for each waste-package type, T_{wp}(DMTH; x,y, waste-package type). This is calculated by adding the temperature variation at the waste package from Step 2, ΔT_{wp}(DDT;

waste-package type), to the abstracted temperature for an LMTH model, T_{dw}(LMTH; x,y) obtained in Step 3. This step determines the distribution of waste-package temperature as a function of waste-package type and location in the repository. The result of this step is assumed to be comparable to having a DMTH-model prediction of the T_{wp} distribution in the repository for each waste-package type; hence the resulting distribution is called T_{wp}(DMTH; x,y, waste-package type), where x and y refer to the coordinate location in the repository. The waste package temperature including hydrology and waste package variability at any repository location is:

$$T_{wp}(\text{DMTH}; x, y, \text{waste package} - \text{type}) = T_{dw}(\text{LMTH}; x, y) + \Delta T_{wp}(\text{DDT; waste package - type})$$

or,

the result of Step 6 = the result of Step 3 + a result of Step 2

Step 7—Determine the Distribution of Relative Humidity on Waste Packages for Each Waste-Package Type

The final step is to determine the distribution of relative humidity on waste packages throughout the repository area for each waste-package type. Note that this step is carried out differently for cases with engineered backfill than it is for cases with no backfill.

For cases with no backfill, relative humidity on waste packages is determined using the drift-wall temperature T_{dw} distribution from Step 4, the drift-wall relative humidity RH_{dw} distribution from Step 5, the waste-package temperature T_{wp} distribution from Step 6, and the relation $RH_{wp} = RH_{dw}[P_{sat}(T_{dw})/P_{sat}(T_{wp})]$, where P_{sat} is the saturated vapor pressure. This relationship assumes that the vapor pressure is constant in the open emplacement drift. The result of this step is the DMTH-predicted waste-package relative humidity distribution, RH_{wp}(DMTH; x,y, waste-package type), calculated using the abstracted drift-wall temperature T_{dw}(DMTH; x,y, waste-package type), the abstracted waste-package temperature T_{wp}(DMTH; x,y, waste-package type), and the relation $RH_{wp} = RH_{dw}[P_{sat}(T_{dw})/P_{sat}(T_{wp})]$. The result of this step is assumed to be comparable to having a DMTH-model prediction of the RH_{wp} distribution in the repository for each waste-package type; hence the resulting distribution is called RH_{wp} (DMTH; x,y, waste-package type), where x and y refer to the coordinate location in the repository.

For cases with engineered backfill, relative humidity on waste packages cannot be determined from the relation $RH_{wp} = RH_{dw}[P_{sat}(T_{dw})/P_{sat}(T_{wp})]$ because of the influence of capillary-driven wicking in the backfill. Thus, the influence of TH behavior in the backfill must be accounted for in this step. This step requires the local-temperature difference between the waste package and drift wall $\Delta T_{wp,local}$(DDT; waste-package type) for each waste-package type and the scanning curves for RH_{ratio}(LDTH) vs. ΔT_{bf}(LDTH) from Step 2. This step also involves spatial interpolation among the 35 locations and interpolation among the three AML scanning curves in (Figure 3-50g) on the basis of $\Delta T_{wp,local}$(DDT; waste-package type). The result of this step is assumed to be comparable to having a DMTH-model prediction of the RH_{wp} distribution in the repository for each waste-package type; hence the resulting distribution is called RH_{wp} (DMTH; x,y, waste-package type), where x and y refer to the coordinate location in the repository.

3.5.4.2.2 Constructing Probability Density Functions of Engineered-Barrier System Thermal-Hydrologic Conditions

Predictions from the TH multiscale modeling and abstraction method are used by several modeling and analysis groups that support TSPA-VA:

- Waste-package corrosion
- NFE geochemistry
- Waste-form dissolution
- Transport of radionuclides through the engineered barriers.

It is possible to provide the full set of TSPA-VA performance measures (Table 3-9) for all seven major waste-package types (Table 3-22) at every waste-package location in the repository area. However, because it is unfeasible to perform the necessary calculations for all four of the listed groups, it is necessary to group waste-package environmental conditions into "bins."

For waste-package corrosion analysis, the process of "binning" the waste-package environments involves several steps. First, the repository area is subdivided into six major subdomains with respect to infiltration flux q_{inf}, using the infiltration map in (Flint et al. 1996a). The boundaries between the subdomains (Figure 3-52) are chosen to minimize the variability of q_{inf} within each subdomain. Thus, there are low-q_{inf} subdomains and high-q_{inf} subdomains. The rationale for grouping the waste-package environments into these subdomains is that q_{inf} is a major factor in determining how long and whether conditions during the thermal period are relatively hot and dry or cool and humid. For purposes of drift-seepage modeling, q_{inf} is a major factor determining the tendency for water to seep into emplacement drifts. The six q_{inf} subdomains correspond to the northeast and northwest corners of the repository area, the central region, the south-central region, and the southwest and southeast corners of the repository area.

The second step for binning waste package environmental conditions is to group the five CSNF waste-package types into a single CSNF waste-package category and to group the co-disposal HLW packages with the separate-disposal DOE SNF waste packages into a single HLW-package category.

The third and fourth steps of binning involve developing probability density functions of temperature and relative humidity conditions for the CSNF waste-package category and for the HLW-package category in each of the six q_{inf} subdomains. The probability density functions are expressed as relative humidity and temperature histograms. The environmental conditions on waste packages are binned according to the time required by waste packages to return to relative humidity = 85% and to temperature on the waste-package surface at 5,000 year. A relative humidity of 85% was selected because it is a typical of the critical relative humidity for atmospheric corrosion (RH_{crit}) (i.e., the value of relative humidity where atmospheric corrosion is initiated). Once $RH > RH_{crit}$, the corrosion rate for the outer corrosion-allowance material on the waste package also depends on temperature at the waste-package surface. Because the relative humidity generally exceeds 85% within 5,000 years (unless an engineered backfill is used), temperature at 5,000 years is a good indicator of whether the waste-package environment is relatively hot or relatively cool when humidity returns to 85%.

In each of the repository subdomains based on infiltration flux, the CSNF and HLW-package categories are grouped into ten relative-humidity bins, and each relative-humidity bin is subdivided into three temperature bins, resulting in a total of 30 bins for CSNF waste packages and 30 bins for HLW packages. For example, if all waste packages attain relative humidity = 85% within 3,000 years, the waste packages could then be subdivided into groups where relative humidity = 85% is attained within 0 to 300 years, 300 to 600 years, and so on, with the last relative-humidity bin containing waste packages that attain relative humidity = 85% from 2,700 to 3,000 years. Step 3 of the binning process is complete when all of the waste packages have been placed in their respective relative-humidity bins.

Step 4 of the waste-package environment-binning process involves subdividing the waste packages in a given relative-humidity bin group into three temperature bins, corresponding to temperature on the waste package at 5,000 years. After completing Step 4, all CSNF waste packages and all HLW packages will fall somewhere within their respective 30 relative humidity and temperature bins. The sum of the probabilities for the 30 bins will be 100%, for both CSNF relative humidity and temperature and for both HLW relative humidity and temperature. It is possible for many of the relative-humidity and temperature bins to contain no waste packages.

Step 5 of the binning process involves selecting a typical waste-package location for each of the 30 bins that contains a non-zero probability. The mean rewetting time (to relative humidity = 85%) and the mean temperature at 5,000 years is calculated for all waste packages in a relative-humidity and temperature bin. Least-squares minimization is used to find the waste-package location that is closest to having the mean relative-humidity = 85% rewetting time and the mean temperature at 5,000 years. The temperature and relative-humidity histories for the typical waste package within each bin, along with the probabilities for each of the relative-humidity and temperature bins, are provided to TSPA-VA for waste-package corrosion analysis. The other NFE conditions listed as performance measures in Table 3-9 are also provided to TSPA-VA for each of these typical waste packages.

The procedure used for binning near-field conditions for geochemistry analysis is identical to that described above for the waste package corrosion analysis. In this case we want to select the typical waste package from the bin containing the median waste package. As before, the bins are created by determining, for each waste package, the time at which the relative humidity reaches 85% and the temperature at 5000 years. The typical waste package is selected by calculating a normalized (with respect to the bin averaged temperature at 5000 years and the bin averaged time to 85% relative humidity) least squares minimization for the median waste package. This procedure is repeated for the HLW-package group. A full set of NFE conditions, including the liquid-phase saturation in the invert $S_{liq,inv}$ is provided to TSPA-VA for the typical CSNF waste package and the typical HLW package in each of the six q_{inf} subdomains. This information is also used by the groups analyzing waste-form dissolution and analyzing transport in the engineered barriers.

3.5.5 Base-Case Results

3.5.5.1 Base-Case Mountain-Scale Results

Air Mass Fractions and Gas-Flow Rates

The air mass fractions and the gas-flow rates are used in the near-field geochemistry models. The amount of CO_2 that exists near the repository can affect the degradation rate of the concrete in the liner or in the invert as well as alter the pH of the water near the repository. Any oxygen present near the waste form will be available to oxidize the waste form. Consequently, the presence or absence of CO_2 and O_2 as well as the rate at which they are replenished can impact the performance of the repository.

The air mass fraction and the gas fluxes in the repository were generated using the two-dimensional G-ECM mountain-scale, TH model. All of the rock property sets were run at both the present-day and long-term average infiltration rates over the cross section located at northing = 233,400 m. The air mass fraction and gas-flow rates were found at both the center and the edge of the repository. The "center" location was at easting = 170,650 m and the "edge" location was at easting = 171,200 m. The form of the information given to the near-field geochemistry is a table that contained time, air mass fractions, and gas-phase fluxes flowing thorough the four sides of the "center" and "edge" repository element. To make it easier to compare the magnitude of gas fluxes from one simulation to another, the gas-phase fluxes over all four sides of the repository elements have been averaged. In this model, each of the repository elements in the two-dimensional model was 6 meters high and 25 meters wide.

The air mass fraction in the repository element will change as different mechanisms either drive air away from the drift or permit air to return. Initially, the steam that is generated by the waste packages drives water vapor and air away from the repository resulting in a drop in the air mass fraction. As the rocks surrounding the element dryout, this water-vapor flux diminishes, allowing air to diffuse back to the repository. As the waste packages cool off, water that had been accumulating above the repository, can imbibe into the rocks near the repository. Some of this water can then vaporize as it cools the hot rock resulting in the air mass fraction dropping a second time. As the heat output from the waste packages drops to zero, the air mass fraction around the repository will eventually return to the ambient value of 0.98.

Figures 3-53 through 3-58 show the expanding and contracting steam zone from 30 to 10,000 years for the α_f mean base-case property set at present-day infiltration conditions. The vectors that are superimposed on the temperature field represent the gas-flow rates. The length of the vector at the bottom of the figures represent a gas flux of 5.0×10^{-6} kg/m^{2}s. The scale of the gas flux vectors plotted in the figures is the same. Large-scale gas-phase re-circulation regions do not develop in the UZ. This is because the vertical permeabilities are larger than the horizontal permeabilities, resulting in flows that are primarily in the vertical direction. Although the air mass fractions are not presented in the figures, an estimate of the air mass fraction field can be found by assuming that the air mass fraction is inversely related to the temperature.

The air mass fractions in the element located at the center of the repository for the five base-case runs at present day infiltration rates are presented in Figure 3-59. The infiltration rates over the

cross-section are 2.65 mm/year (I÷3), 7.96 mm/year (nominal I), and 23.9 mm/year(I*3). The first minimum air mass fraction of between 10^{-7} and 10^{-6} was reached for all five simulations between 30 and 50 years. The minimum air mass fraction for two cases with the higher infiltration rates had a lower minimum and it happened later than for the other three cases. After reaching this minimum, the air mass fractions began to rise until, at 150 years, the air mass fractions fell due to evaporation of the water imbibing back near the repository. The air mass fractions began to rise between 600 and 900 and reached 0.2 after 2,000 years.

The air mass fractions at the eastern edge of the repository (Figure 3-60) did not show much variability. The minimum air mass fraction of approximately 10^{-3} occurred at 30 years. At 150 years, the air mass fraction reached 10% in all five simulations. After 2,000 years, the air mass fractions reached 0.50.

These results show that, for the range of simulations carried out, the air mass fractions are more sensitive to the location in the repository than α_f or the variation in present-day infiltration rates that were contained in the base-case property sets.

The air mass fractions in the element located at the center of the repository for the five base-case runs at the long-term average infiltration rates are presented in Figure 3-61. The infiltration rates over the cross section are 15.1 mm/year, 45.3 mm/year, and 136 mm/year. The air mass fraction time-histories for the one-third of long-term average and the long-term-average property sets showed similar to those at the present-day infiltration. The air mass fraction time-histories for the three times the long-term-average infiltration rate case did not have the second minimum at 700 years. The results show that, for the base-case parameter sets during long-term-average climate conditions, the air mass fraction appears to be much more sensitive to the variability in infiltration rate than it is to the variability in fracture van Genuchten α_f.

The air mass fractions at the eastern edge of the repository for the five base-case runs at long-term-average infiltration rates are presented in Figure 3-62. As in the case at present-day climate conditions, the air mass fractions are not substantially different between base-case property sets.

Although it is clear that the infiltration rates seem to have a greater difference in air mass fraction behavior than does α_f, the differences between air mass fraction time-histories at the center and at the edge of the mountain is still much more important than the infiltration rates.

The gas flux at the center of the repository for the base-case property sets at present-day climate conditions is presented in Figure 3-63. The gas flux peaks at $\sim 3 \times 10^{-6}$ kg/m^{2}s between 10 and 20 years. This peak is just over an order of magnitude larger than the gas-phase flux after 10,000 years. The behavior for the curves are quite similar except for a drop in the gas-flow rates between 300 and 800 years for the two low infiltration cases. The drop in the gas-flow rates for the low infiltration simulations was due to local dryout in the repository element. The drop in gas flux coincided with the drop in the air mass fraction resulting in a small change in the amount of CO_2 available in the drift to react with the concrete.

The gas flux at the edge of the repository for the base-case property sets at present-day climate conditions are presented in Figure 3-64. As is the case for the center of the repository, the gas flux peaks at $\sim 3 \times 10^{-6}$ kg/m^{2}s between 10 and 20 years. The gas fluxes for all of the base-case

property sets overlap for the first 3,000 years after which the higher infiltration simulations have slightly lower fluxes.

The gas flux at the center of the repository for the base-case property sets at the long-term average climate conditions are presented in Figure 3-65. The five base-case simulations showed similar behavior for the first 1,000 years. The gas fluxes peaked at ~3×10^{-6} kg/m^{2}s between 20 and 30 years and dropped to at ~3×10^{-7} kg/m^{2}s at 1,000 years. From 1,000 to 3,000 years, the gas fluxes for the two high-infiltration cases (long-term-average I*3) dropped to ~1×10^{-9} kg/m^{2}s. The gas fluxes for these cases stayed at ~1×10^{-9} kg/m^{2}s for the duration of the simulation. The gas fluxes for the other three simulations using the long-term-average infiltration rate were similar to those from the present-day infiltration cases.

The gas flux at the edge of the repository for the base-case property sets at the long-term-average climate conditions are presented in Figure 3-66. The gas-phase flux curves were similar in shape to the profiles from the present-day infiltration cases. From 200 to 2,000 years, the gas fluxes for the highest infiltration rate cases were a third of a magnitude lower than the gas fluxes for the other three cases.

As is the case for the air mass fraction time histories, the difference between center and edge behavior was much larger than any variation caused by using the different property sets.

3.5.5.2 Base-Case Drift-Scale Results

The base-case TH results for TSPA-VA are presented at the scale of the drift as computed from the TH multiscale modeling and abstraction method described in detail in Sections 3.5.1 and 3.5.4. This section provides temperature and relative-humidity results, at the surface of the waste package, for the base-case thermal and hydrologic property sets described in Section 3.5.2 and the reference repository design described in Section 3.5.3. Most of the results presented here are for the base-case property sets. Some comparisons include results from additional property sets compared directly to the base case in order to illustrate specific points. The following descriptions indicate TH response with respect to hydrologic property uncertainty as well as infiltration-rate uncertainty. Thermal-hydrologic uncertainty, incorporated into the analysis through the use of a "thermal-hydrologic property set," is also compared to base case in the form of average waste-package-temperature predictions at repository subregions NE and SW.

Temperature and Relative Humidity

Figure 3-67 and Figure 3-68 display variability in average waste-package temperature among the six repository subregions for the nominal (mean) I infiltration rate and mean fracture alpha case (for example, DTN LB971212001254.001). Figure 3-67 indicates the long-term-average climate; Figure 3-68 indicates the present-day climate. The early behavior, when temperature is increasing, is largely influenced by the infiltration rates, the initial liquid saturation of the host rock, and the host-rock thermal properties, in particular, the thermal conductivities. The thermal conductivity varies from repository subregion to subregion depending on whether or not the repository-host unit falls within a lithophysal unit. For regions located in the lithophysal zones, in particular at low infiltration rates, the initial heat up is more rapid than at other locations. Consider the following describing average waste-package temperatures obtained for different

repository subregions. Region SW is located in the Topopah Spring Lower Nonlithophysal unit (Tptpln), region SE is located partially in the Topopah Spring Middle Nonlithophysal unit (Tptpmn) and the Topopah Spring Lower Lithophysal unit (Tptpll), and region CC is located entirely in the Topopah Spring Lower Lithophysal unit (Tptpll). The LTA infiltration rates for the subregions are 32, 33, and 55 mm/year, respectively. Initial heating indicates that region SW heats up faster than SE or CC. Region SW has the lowest infiltration rate as well as the lowest wet-value thermal conductivity; therefore, its temperatures are highest. As the maximum temperature is reached, and drying of host rock occurs, region SE overtakes SW since the lithophysal dry-value thermal conductivity is the lowest in the repository host unit. Region CC heats up the slowest since it is subjected to the highest infiltration rate. Edge response is not a factor at early times; however, during cooldown, preferential cooling for subregions close to the repository edge becomes increasingly noticeable with time. Subregion SW cools off the fastest because all of it is near the repository edge. Subregion CC cools off the slowest because it is the only interior subregion and therefore is farthest from the repository edges. After 10,000 years, little variability remains from subregion to subregion. This is important since most waste package failures occur after a time when most of the subregions behave nearly identically with respect to the thermal hydrology.

Figure 3-67 illustrates temperatures calculated as if the long-term-average climate (see Section 2.4.1 in Chapter 2 of the TSPA-VA Technical Basis Document) were in effect throughout the entire period (average infiltration of about 40 mm/year over the entire repository). In reality, the TSPA-VA climate model includes cycling between dryer (present-day average infiltration) and wetter (long-term-average) climate states. Climate effects on TH are included by making two sets of calculations, one with present-day climate for the entire period and one with long-term-average climate for the entire period. The influence of climate change on TH behavior is then approximated by switching from one set of results to the other at the time of climate change. This approximation was tested against simulations in which infiltration was varied through time, and the response to changes in infiltration was found to be fast enough that the approximation can be used (refer to Section 3.4.4). Figure 3-68 illustrates temperatures calculated as if the present-day climate were in effect throughout the entire period (average infiltration of about 8 mm/year). Temperatures for present-day climates are slightly higher (higher infiltration lowers repository temperature because of the influx of cooler infiltrating water at the ground surface). Only the first climate change, between 1,000 and 10,000 years, is relevant to TH; by the second climate change, between 80,000 years and 110,000 years, temperatures and relative humidities have essentially returned to ambient conditions. Although the illustrations here are for CSNF waste packages, the results for HLW and separate-disposal DOE spent fuel are qualitatively similar.

Figure 3-69 is the correspondent relative humidity response for the long-term-average temperature curves given in Figure 3-67. The curves represent the average relative humidity, at the waste package surface, from subregion to subregion for each of the six repository regions. The repository center (region CC) produces lower relative humidities than subregions with proximity to the repository edges. Edge relative humidity increases as heat is lost to the surrounding rock mass and the temperatures inside the drifts are reduced.

Figure 3-70 and Figure 3-71 show the variability of waste-package temperature and relative humidity within one of the repository subregions (Region NE). The variability results primarily

from the variability in heat output among waste packages and to a lesser extent from variability in infiltration and stratigraphy within the subregion. The influence of decay heat is negligibly small after 100,000 years. As indicated in Figure 3-70 some of the hotter waste packages maintain boiling temperatures for 1,000 to approximately 4,000 years. Other waste packages proceed below the nominal boiling point in the first 100 to 1,000 years after waste emplacement. The fact that the temperature predictions do not significantly flatten at the nominal boiling is a result of the dual permeability model applied in the TH multiscale modeling and abstraction method.

Figure 3-72 shows how average waste-package temperature is affected by the potential variability in UZ flow (both in hydrologic properties and in infiltration rate) incorporated into the TSPA-VA base case. This comparison is for long-term-average climate and it includes TH results for DTN LB971212001254.001, DTN LB971212001254.002, DTN LB971212001254.003, DTN LB971212001254.004, and DTN LB971212001254.005 hydrologic property sets (all not qualified). The results are shown only for the repository subregion NE. Other subregions are analogous. For subregion NE, the high-infiltration cases (~90 mm/year) have cooler temperatures than the mean-infiltration (~30 mm/year) or low-infiltration (~10 mm/year) cases. This figure shows that the TH variability associated with potential variability in infiltration rate dominates the variability associated with uncertainty in hydrologic properties.

Figure 3-73 and Figure 3-74 show how waste-package temperature is affected by additional uncertainty in hydrologic-properties beyond those included in the base case. Of particular importance in this section is the hydrologic-property set developed in order to quantify TH uncertainties in the processes occurring during drying and subsequent rewetting. The "thermal-hydrologic property set" is different from the base-case hydrologic properties primarily in having a much lower imbibition diffusivity for the rock matrix of the Topopah Spring Lower Nonlithophysal hydrogeologic unit, a change suggested by results of the single-heater test. Figure 3-73 is for repository subregion SW; Figure 3-74 is for repository subregion NE. Figure 3-73 indicates that early time behavior (approximately the first 100 years) is somewhat different between hydrologic property sets for region SW. The "thermal-hydrologic property set" indicates rapid initial heating when compared to the base-case results. This repository subregion resides in the Topopah Spring Lower Nonlithophysal hydrogeologic unit (Tptpln). The unit directly below this also has reduced matrix imbibition diffusivity (Tptpv). As a result, a more pronounced superheating region occurs as indicated by higher temperatures. This property set results in higher temperatures (and hence lower relative humidities) for approximately 10,000 years after waste emplacement. After 10,000 years, any differences are considered negligible. A comparison is also made for a repository subregion located partially in the Topopah Spring Middle Nonlithophysal hydrogeologic unit (Tptpmn) and the Topopah Spring Lower Lithophysal hydrogeologic unit (Tptpll) shown in Figure 3-74. However, because the repository horizon located in subregion NE is far from the Topopah Spring Lower Nonlithophysal hydrogeologic unit, we expect to see little sensitivity of TH behavior to this change in hydrologic properties. This is the case. Because the repository horizon in subregion SW occurs within the Topopah Spring Lower Nonlithophysal, we would expect to see much greater dependence of the TH behavior on this change in hydrologic properties. Heater tests in the east-west cross drift could aid in determining the dependence of the TH behavior.

Figure 3-75 through Figure 3-78 indicate average temperature response curves for each of the repository subregions for the end members of the base-case hydrologic property set. That is, maximum α_f, I*3 and minimum α_f, I/3 infiltration rates. Both the present-day and long-term-average climate states are included. For maximum α_f, I*3, the average infiltration rate for the present day is approximately 23 mm/year while the average infiltration rate for the long-term-average climate is approximately 126 mm/year. For minimum α_f, I/3, the average infiltration rate for the present day is approximately 3 mm/year while the average infiltration rate for the long-term-average climate is approximately 14 mm/year. Reference to Figure 3-72 indicated that the TH response to hydrologic property uncertainty in fracture alpha (α_f) is overwhelmed by the uncertainty in infiltration rate; hence, these figures indicate the *largest potential variability* in average waste-package temperature for each of the repository subregions considered in TSPA-VA. Figure 3-78 indicates the highest possible temperatures resulting from the base-case hydrologic property set (average present-day I/3 infiltration rate approximately 3 mm/year). Figure 3-75 indicates the lowest possible temperatures resulting from the base-case hydrologic property set (average long-term-average I*3 infiltration rate approximately 126 mm/year). In order to more readily see the effect of this uncertainty, Figure 3-79 displays the largest potential variability in temperature occurring within repository subregion NE for the end members of the base-case property set. The figures above represent the major influence of UZ flow uncertainty on TH. As indicated in previous figures, the hydrologic property uncertainty is overwhelmed by the uncertainty in infiltration rate with subsequent climate changes. Figure 3-79 includes maximum infiltration rate variability with climate change imposed. In order to see the influence of climate change alone, consider the following figures.

Figure 3-80 indicates the average temperature and relative humidity for repository subregion NE using the mean α_f and nominal (mean) I case. The present-day and long-term-average climate states are considered so that one can see the TH response resulting from climate change only. From the figure the long-term-average climate produces lower temperatures and higher relative humidities. It is a result of lower temperature water washing into the repository horizon at a much higher flow rate from the ground surface. It is a convective cooling process that suppresses temperature and increases relative humidity. After 1,000 years, the percent change in relative humidity is about 12.5% higher for the long-term-average case and the temperature is approaching the nominal boiling point. At the present-day climate, the temperatures are still above the boiling point 1,000 years after waste emplacement.

All of the results shown above are for individual or average CSNF waste packages. The CSNF waste packages represent approximately 75% of the entire repository inventory. Recall from Section 3.5.3 that the base-case drift segment in the drift-scale models contain additional waste packages including the HLW and the separate-disposal DOE SNF. The additional waste packages are compared to the commercial waste packages for two repository subregions: NE and SW. Figure 3-81 indicates the average waste package temperatures and relative humidities for subregion NE. Figure 3-82 indicates the average temperatures for subregion SW. The variability between the commercial fuel and the additional waste, on average, is not very large for these subregions. This is due mainly to the placement of the co-disposal waste package (approximately 4 kW) between the larger and hotter 21 PWR waste packages. Recall that a spacing criterion between commercial and additional wastes (minimum 1-m separation distance) constrained the placement of the co-disposal waste package between the design-basis waste

package and an average heat output 21 PWR waste package. The design-basis waste-package heat output is approximately 18 kW while the average 21 PWR is approximately 9 kW. This (co-disposal) waste package could not be placed next to the colder 21 PWR or the 12 PWR because there were space limitations. Recall that the reference-repository design is for an open emplacement drift. Radiant heat transfer effectively spreads energy between closely spaced waste packages ultimately raising the temperatures of the waste packages producing lower thermal outputs. If rockfall or backfill occurs, the results would be altered since there is much less sharing of heat between waste packages since each acts as a point source of energy covered by fill. One alternative location for this waste package would be between the interior 44 BWRs (the exterior already contains the direct-disposal waste package). Although the direct-disposal waste package initially is at a very low power output, it only represents approximately 33% of the additional waste packages in the repository and in the drift segment. Therefore, the results of the co-disposal waste package appear to drive the response curves for the additional wastes.

As discussed earlier, the environmental conditions on waste packages are binned according to the time required by waste packages to return to a relative humidity of 85%. A relative humidity of 85% was selected because it is a typical of the critical relative humidity for atmospheric corrosion (RH_{crit}) (i.e., the value of relative humidity where atmospheric corrosion is initiated). A useful way to display the distribution of environmental conditions on all waste packages throughout the repository is to use a complementary cumulative density function (CCDF) of the time required for waste packages to rewet to an relative humidity of 85% (Figure 3-83). The CCDF of waste package rewetting time is affected by three key factors:

- Edge-cooling effects, with waste packages closest to the repository edges cooling earlier, this causes them to rewet earlier than waste packages closer to the repository center. There is a gradual progression from edge-like rewetting times to center-like rewetting times.

- Repository-scale variability of percolation flux, with waste packages in areas of high percolation flux rewetting earlier than waste packages in areas of lower percolation flux. (Recall that because of the assumption that spatial attenuation of infiltration flux is negligible, the percolation-flux distribution and infiltration-flux distribution are equivalent.) The wide range of infiltration (and percolation) flux in the repository area results in a wide range of waste-package rewetting times.

- Waste package-to-waste package variability of heat output, with cooler waste packages rewetting earlier than hotter waste packages. Because of the wide range of waste package heat output, there is a wide range of waste package rewetting times. For cases with engineered backfill, this factor dominates the CCDF of waste package rewetting times, particularly for the quartz-sand-backfilled, point-load design.

The CCDF of waste-package rewetting time is also affected (to a somewhat lesser extent) by a fourth factor:

- Matrix imbibition diffusivity $D_{imb,m}$ of the local host rock, which is a measure of the magnitude of capillary-driven rewetting in the rock matrix, with waste packages in regions of high $D_{imb,m}$ rewetting earlier than waste packages in regions of lower $D_{imb,m}$.

Because the tsw36 (Tptpln) host-rock unit has a much higher $D_{imb,m}$ than the tsw34 and tsw35 (Tptpmn and Tptpll) host-rock units, waste packages lying in the tsw36 tend to rewet earlier.

The TSPA-VA base-case family of hydrological property sets includes five property sets: (1) $\alpha_{f,mean}$, (2) $\alpha_{f,min}$, I x 3, (3) $\alpha_{f,max}$, I ÷ 3, (4) $\alpha_{f,min}$, I x 3, and (5) $\alpha_{f,max}$, I x 3, where I stands for the nominal infiltration-flux map and α_f stands for the van Genuchten "alpha" parameter for fractures. These property sets are applied to five cases that assume the present-day-climate (I) infiltration-flux map and to five cases that assume the LTA infiltration-flux map. Figure 3-83 plots the CCDF of waste package rewetting time for all ten of these cases for the point-load design with no backfill.

The magnitude of percolation flux significantly affects the magnitude of rewetting times, but it does not affect the overall shape of the CCDF of waste package rewetting times (Figure 3-83). A factor-of-three decrease in percolation flux results in a 40% increase in rewetting time for the median waste-package, while a threefold increase in percolation flux results in a 40% decrease in rewetting time for the median waste-package. The influence of the range of α_f that was considered is not as strong as a threefold difference in infiltration flux. For the I ÷ 3 cases, the rewetting time for the median waste package is 6% greater for the $\alpha_{f,min}$ case than it is for the $\alpha_{f,max}$ case, while for the I x 3 cases, the rewetting time for the median waste package is 15% greater for the $\alpha_{f,min}$ case than it is for the $\alpha_{f,max}$ case. For the LTA x 3 cases, the influence of α_f is much stronger than it is for the LTA ÷ 3 cases.

3.5.6 Interpretation of Results

3.5.6.1 Base-Case Mountain-Scale Results

The air mass fraction and gas flux obtained by the two-dimensional mountain-scale TH models provides the near-field geochemistry model (Chapter 4, TSPA-VA Technical Basis Document) the information needed to compute the quantity of O_2 available to oxidize the waste packages and the quantity of CO_2 available to carbonate the concrete in the drift. In order to limit the amount of O_2 and CO_2 in the drift, it would be advantageous to keep the air mass fraction and gas-flow rates as low as possible for as long as possible.

The air mass fraction and gas-flux time-histories were solved for at both center and edge locations. As a first-order approximation, the quantity of O_2 and CO_2 in the gas phase is equal to the product of the air mass fraction, the gas flux, and the mass fraction of the gas (O_2 or CO_2) in air. The gas-flux time-histories at the center and the edge were similar for the first 1,000 years and then the gas flux at the center was up to ten times higher than that at the edge after 1,000 years. The air mass fraction time-histories at the edge were always higher than the air mass fraction at the center of the repository. A consequence of this is that more O_2 and CO_2 will flow through the edge rather than the center of the repository when the repository is hot, but more O_2 and CO_2 will flow through the center rather than the edge of the repository when the repository has cooled down.

3.5.6.2 Base-Case Drift-Scale Results

The results (presented in the previous section) obtained from the TH multiscale modeling and abstraction method provide the necessary information that governs the thermodynamic response in the EBS and within the altered zone. The altered zone is created and driven by the heat component of the emplacement waste. The heat component drives processes that increase temperature, decrease relative humidity, transport water vapor, dry rock, create condensate flow, and alter the ambient-flow properties of the mountain surrounding the waste for many thousands of years after waste emplacement. Temperature and relative-humidity curves indicate the environment inside the drift near the waste packages. They drive the response of the waste packages to a corrosive environment. Waste-package temperature and relative-humidity response curves, as shown in the previous section, are input into waste-package corrosion models, such as WAPDEG (refer to Chapter 5, TSPA-VA Technical Basis Document), which predict the overall lifetime of a waste package in a repository drift. With the specification of a threshold temperature, a relative-humidity threshold for humid-air corrosion, a relative-humidity threshold for aqueous corrosion, and information related to dripping rate and fraction contacted, the corrosion processes related to humid air general corrosion, aqueous general corrosion, and aqueous pitting corrosion can be quantified so as to describe the corrosion rates of the outer corrosion allowance material (CAM). The TH models developed for TSPA-VA supply threshold values. Corrosion rates of the inner corrosion resistance material (CRM) are a function of temperature among other things. The TH models developed for TSPA-VA supply temperature ranges to the corrosion-rate analysis of the CRM.

The evolution of the thermodynamic environment in the emplacement drift is also applied to the in-drift gas model developed to describe the near-field geochemical environment (see Chapter 4, TSPA-VA Technical Basis Document). As described above in the mountain-scale results, the air-mass fraction and the gas-flux and air-flux evolutions are applied to the gas composition models applied in the near field. Abstracted time periods used in the gas-composition models are driven by the evolution of the drift-wall temperature. The drift-wall temperatures used in the gas-composition model resulted from the TH multiscale modeling and abstraction method. The abstracted gas-composition models are applied to two regimes, boiling and cooling. Each regime contains three abstracted time periods as driven by the average drift-wall temperature. The temperature range is from 95°C to 30°C for the abstracted time periods at which the gas-composition models are applied.

Finally, liquid saturation of the invert material is an important quantity in determining the diffusion coefficient used to transport radionuclides from the waste packages through and out of the EBS (see Chapter 6, TSPA-VA Technical Basis Document). The invert liquid saturation obtained from the TH multiscale modeling and abstraction method is applied directly into RIP. Also, an important aspect of engineered-barrier release is clad breach allowing air and/or water into the waste form. Performance of the repository improves if the clad remains intact. The characterization of the cladding is a function of temperature and mechanical disruptions that may occur in the event of rockfall. The waste-package surface temperature, as computed by the TH multiscale modeling and abstraction method, is applied directly in RIP to determine waste-form degradation processes.

The feeds from TH have been discussed in the above paragraphs. The importance of TH is evident as it drives most of the near-field models used to quantify waste package and waste form lifetimes as well as the gas compositions inside the drift. For the base case, TH has developed a model based on the hydrologic flow properties developed in the UZ flow tasks and a reference-repository design based on most recent repository design information.

The inputs to TH, such as rock properties, infiltration rates, and repository design, drive, to a large extent, the results obtained from the models that include the thermal perturbation resulting from radioactive decay heat. The maximum (peak) temperatures and minimum relative humidities (occurring for most waste packages in the first 15 to 25 years after emplacement) in the drift are explicitly tied to the AML, drift spacing, waste-package heat output, and the thermal and hydrologic properties of the surrounding host rock units. For example, waste emplacement in the lithophysal zones tends to produce rapid heatup since the dry thermal conductivity is low there. The temperature curves (discussed above for the base case) as a whole shift up or down depending on the infiltration-rate boundary condition. The cooldown temperature of the waste packages is very sensitive to the infiltration rates. For times greater than 1,000 years after emplacement, waste-package surface temperatures for the high infiltration rate are about 20°C cooler than the nominal I infiltration rate. The nominal I case is only about 5°C cooler than the lowest infiltration rate cases. (This comparison is for the LTA climate state in effect at all times.)

The infiltration rates vary over each of the repository subregions (NE, ...). The range of average infiltration rate in the repository subregions is 3.9 mm/year to 11 mm/year for the present-day climate. For the LTA climate, that range is from 31 mm/year to 55 mm/year. For lower infiltration rate cases, waste-package temperatures remain above boiling for longer periods of time. Additionally, the period of relative-humidity reduction is extended. For waste packages with dripping at all times, higher temperatures have adverse effects on corrosion. For dry waste packages (no drips) low relative humidity is beneficial with respect to corrosion. For the waste packages seeing drips at all times, the lower infiltration rate (and hence higher predicted temperatures) produced failed waste packages at earlier times. However, overall, the higher infiltration rate cases have more waste packages with drips and hence more overall releases. The extent of dryout produces different TH responses.

The extent and duration of dryout, a function of the heat released to the mountain, but also a function of the imbibition diffusivity characteristics of fractures and matrix rock, dictate the temperature increase as well as the reduction in relative humidity. The formation of a larger dryout zone results in lower thermal conductivity and lower heat capacity in the rock surrounding the waste packages. This in turn drives temperatures up while reducing the relative humidity inside the drift. It also facilitates reduction of drips on waste packages. Other processes related to evaporation and the build-up of pore pressure in the matrix serve to raise the temperatures near the heat-generating sources. The TH property set produces a more extensive dryout zone by reducing the rewetting rates in the host units after cooldown begins. This produces favorable conditions for the waste packages when compared to hydrologic property sets that potentially overestimate the rate of rewetting parameters applies during heating processes. Response of the EBS is a function of waste-package temperature as well as of the liquid saturation evolution of the concrete invert.

Waste-package temperatures influence the contents of the waste packages. For higher temperatures (much higher than those predicted in TH model analyses) clad breach may allow water or air into the waste form. For the waste packages with very high heat output, such as the design-basis-fuel waste packages, it is important that the surface temperatures of the waste packages not produce clad temperatures greater than 350°C. In an empty drift, heat limitations are essentially maintained at all waste packages so that cladding breach resulting from high temperature is not a consideration. Engineered-barrier-system transport is also a function of the invert liquid saturation. The invert liquid saturation results from the TH multiscale modeling and abstraction method. For the matrix hydraulic properties of the concrete used in the TH simulations, rewetting from dried conditions is extremely rapid so that a diffusion coefficient based on a matrix saturation of nearly unity is a conservative result.

The preceding discussions are for the base-case TH results. Sensitivity studies are performed in order to ascertain the uncertainty or potential process variability that results from the conceptual assumptions applied to the base-case models.

3.5.7 Guidance for Sensitivity Studies

The results of the TH processes discussed in the previous sections are specifically for the *base-case* property set (both thermal and hydrologic) and reference-repository design. Hydrologic property uncertainties in the UZ flow models not considered in the base case necessitate additional TH calculations using other, potentially appropriate, hydrologic property sets governing the UZ flow processes occurring at Yucca Mountain. Alternative infiltration rate uncertainty is also incorporated into UZ flow models. In addition to hydrologic properties and infiltration, repository design options and the effects of specified designs (such as an open emplacement drift or a particular waste-package sequence) need also to be considered.

Except for uncertainties associated with repository design (for example, thermal loading, the use of backfill, and waste-package configurations), the TH analyses introduce no new parameter uncertainties to the TSPA-VA analyses. The TH property set is an uncertain parameter set used to describe thermal- and hydrologic-flow processes that occur in response to the emplacement of heat-generating wastes. It does not introduce a new or different form of uncertainty for consideration in TSPA-VA, but it does serve as a means of addressing the uncertainty associated with applying hydrologic property sets to processes (for example, TH) that include complexities far beyond those considered in UZ flow alone. An example of a TH response from this special property set is given in Section 3.5.5 in Figure 3-73 and 3-74. A tacit assumption in TH is that TH calculations can use the same uncertain parameters as the UZ flow component (see Chapter 2, TSPA-VA Technical Basis Document). This property set will help determine if this is valid. Some of the most important of these uncertainties are hydrologic properties, infiltration rates, and future climate states. Examples of how these uncertainties influence TH results for the base case were shown in Section 3.5.5. Examples of how these uncertainties influence TH processes for other hydrologic property sets are described below and in detail in Section 3.6.2.

Additional hydrologic property sets include uncertainty in the intrinsic fracture permeability (minimum, mean, and maximum k_f). This hydrologic property set also includes an interaction parameter between fracture and matrix rock that is proportional to the liquid-phase flow through the fractures. The interaction parameter is proportional to the liquid-phase relative permeability

of the fractures. It is a function of the fracture saturation so that liquid flow is almost entirely restricted to the fractures. This restriction (of water flow only in fractures) may have great impact on the in-drift responses to heat addition. Thermal-hydrologic sensitivity studies using both the TH multiscale modeling and abstraction method and the PA testing models are presented in the upcoming section. Thermal-hydrologic results for the preliminary base case (uses higher infiltration rates) and the TH property set are obtained from the TH multiscale modeling and abstraction method. The DKM/Weeps hydrologic property set (for the mean k_f case only) is also applied in the TH multiscale modeling and abstraction method with results for two repository subregions shown in Figure 3-73 and 3-74 in Section 3.5.5. Additional TH results for the DKM/Weeps hydrologic-property set are obtained using the PA testing models.

In addition to the hydrologic properties, repository design options or the effects of specified designs may serve to alter the TH processes previously described for the base case. If this occurs, waste-package temperatures, relative humidity, drift-wall temperature, and invert liquid saturation can potentially be adversely or positively affected. Potential repository design options include an engineered backfill inserted into the emplacement drift after the mandatory retrieval period has elapsed. Backfill emplacement can potentially serve as a controlled barrier to liquid flow as well as provide for an extended period of a low relative-humidity environment after waste emplacement. As seen in the results presented for the base case, reduction of relative humidity is limited to about 1,000 years or less for most waste packages. Backfill emplacement may aid in providing a dryer environment for the waste packages for longer periods of time. In contrast, if an engineered backfill is not included as an option, as in the reference-repository design, then the potential for drift-wall collapse and a rockfall-rubble-filled emplacement drift should be considered in TH analyses. It is not considered in the base-case results given in Section 3.5.5. The effect of rockfall could easily result in higher waste package temperatures and relative humidities at later times, thus adversely influencing the corrosion rate characteristics of the waste package. An analysis including rockfall processes requires waste-package variability in the emplacement drift segment in order to determine the significance of drift collapse on different waste-package thermal outputs. The results of backfill and rockfall are given in Section 3.6.3 and 3.6.6.

The base-case drift segment described in Section 3.5.3 and applied to the drift-scale models contained different waste-package types (for example, different heat outputs) constrained by waste-stream specifications and a thermal balance with respect to the average repository-wide thermal load. It is further constrained by the AML and the specified emplacement drift spacing. Maintaining the base-case AML and drift spacing, but varying the sequencing of the waste packages (different waste packages with different heat outputs), and hence the thermal output of the drift segment, can result in an assessment of the potential variability that may exist in the predictions made for temperatures and relative humidities of the waste packages. The results of "cold" and "hot" drift segments can quantify the potential uncertainty that exists in waste-package response curves given in Section 3.5.5. A cold-drift segment contains the appropriate waste stream, however, with somewhat colder waste packages of each type. A hot-drift segment also contains the appropriate waste stream, but it contains somewhat hotter waste packages of each type. The results of this analysis are given in Section 3.6.4. This is a waste-stream study at the scale of the waste package. Additional waste-stream studies can also be applied to the scale of the entire repository and mountain.

Mountain-scale analysis in the base case assumed that the entire waste stream is simultaneously emplaced at the time of repository closure. This results in the hottest possible conditions at the time of closure. Predictions for air mass fraction and gas-phase mass flux follow from the solution of the governing conservation equations using an initial condition for the heat output at a maximum. Waste-stream variability and waste aging result in lower initial thermal loads at the time of waste emplacement. The impact of aging the waste is given in Section 3.6.4.

One final recommended sensitivity study is also at the scale of the mountain in the TH analyses. This study considers higher bulk fracture permeabilities in the vertical and horizontal directions in the mountain. It allows for increased rates of gas-phase flow through the mountain after the emplacement of heat-generating wastes. It provides the mountain an even greater ability to "breath." This study serves to determine the gas-phase flow rate influence on the extent and evolution of the air mass fraction at depth. The results of this analysis are given in Section 3.6.7.

The results of base-case TH given in Section 3.5 presume that coupled processes are negligible. This assumption is made partly because there were time limitations in which base-case calculations occurred, but it is also because there was a lack of data and more importantly because of the inherent complexity of any model attempting to include these processes in a fully coupled format. TSPA-VA TH sensitivity analyses considered "coupled processes," or the coupled effects of temperature, hydrology, mechanics, and chemistry in a simplified format so as to assess the potential importance of a particular process on hydrology. When heated, the rock around the emplacement drifts expands. This thermal expansion causes fractures to open and close, which in turn changes the permeability and porosity of the rock and affects movement of both gas and liquid. These changes last only while the rock is heated. In addition, the thermal stresses can cause rock blocks to move and new fractures to form, which again can affect permeability, porosity, and fluid flow. Unlike the simple thermal-expansion effects, these changes to the hydrologic properties of the rock can be permanent. All of these effects are called THM coupled processes. Heating also can cause many chemical changes in rock, such as mineral dissolution in some regions and mineral reprecipitation elsewhere. Mineral dissolution and precipitation can permanently alter the hydrologic properties of the rock, which in turn alters fluid flow. These effects are referred to as THC coupled processes. The initial coupled processes sensitivity studies for mechanical or chemical affects on hydrology are given in Section 3.6.8.

3.6 SENSITIVITY STUDIES

3.6.1 A Testing Analysis Used to Verify the TH Multiscale Modeling and Abstraction Method

The TH multiscale modeling and abstraction method (described in Section 3.5.1) is a complex modeling process involving multiscales (mountain and drift), multidimensions (one, two, and three dimensions), and varying assumptions regarding the coupling of heat transfer to fluid flow (conduction-only and full TH). In order to instill greater confidence that the abstraction modeling approach described in Section 3.5.1 represents the TH processes expected to occur at Yucca Mountain, PA developed independent testing models that include the highest model dimension (three) and fully coupled heat transfer and fluid flow at the scale of the drift. It uses abstracted data from mountain-scale TH models in order to approximate edge effects and it

includes waste-package-to-waste-package variability. It provides predictions at different repository locations and hence includes infiltration rate variability. The drift-scale model used for testing purposes is nearly identical to the DDT model described in Section 3.5.1. However, it includes the TH associated with the problem. The DDT model, as previously indicated, assumes a conduction-only model for heat flow through the mountain. It is clearly noted that the computational requirements of the verification model would not lend itself to the multiple abstraction simulations that are required of a total system calculation. However, models of this type provide an excellent check on the abstraction processes previously described. Good agreement was found when the independent approaches were compared at repository center and edge locations. This comparative analysis addresses the importance of the trade-off between models of different dimensionality. This is a key issue identified by the TH workshop participants.

The TH multiscale modeling and abstraction method described in detail in Section 3.5.1 has been independently checked and verified using three-dimensional TH drift-scale models developed for repository "center" and "edge." Repository-edge models are based on scaling factors obtained from two-dimensional TH mountain-scale models using the solution-matching technique described in CRWMS M&O (1995, pp. 4-13). Waste package (surface) temperature and relative humidity are compared for different waste-package types in the idealized emplacement drift segment described in Section 3.5.3. The comparison study is for an 85 MTU/acre point-load reference repository design. It uses the present-day climate state and the preliminary base-case hydrologic property set. The data-tracking information for this hydrologic property set is the following.

The preliminary base-case property set technical-data information is given in Table 3-3 and is repeated here for convenience. For the nominal I property set, the DTN is LB971100001254.002; for nominal I times 5, the DTN is LB971100001254.001; and for nominal I divided by 5, the DTN is LB971100001254.003. The infiltration rate ranges of multiplied and divided by five are discussed in the UZ flow analyses in Section 2.6.1.1 in Chapter 2 of the Technical Basis Document. Each of the hydrologic-property sets listed above and used in this sensitivity and model verification study is qualified data. The thermal-property data used in this comparison are the base-case values. The development of thermal-property data is found in DTN: SNT05071897001.002. These are unqualified data as specified in Section 3.5.2.

Process-level model uncertainties include both parameter and conceptual-model uncertainty. Parameter uncertainty arises from imperfect knowledge of property variables and the measurement techniques used to obtain them. In this comparative study, parameter uncertainty is de-emphasized by using identical hydrologic and thermal properties applied to each model formulation. The comparative study emphasizes more the differences in conceptualizations applied to each of model formulations. Although more than one difference occurs, the overall driving processes are identical so that a high-level assessment can indeed be made. Model similarities in this comparison study are listed as follows.

The TH multiscale modeling and abstraction method (described in Section 3.5.1) and the PA testing models contain identical input parameters associated with both property sets and repository design data. This includes consistent use of thermal and hydrologic properties

identified above for each of the hydrogeologic model layers taken from the UZ-flow site-scale model. Additionally, reference repository design characteristics such as AML, drift spacing, waste-package spacing and geometry, waste-package types, heat decay curves, and emplacement drift geometry are the same. Finally, identical infiltration-rate boundary conditions at the model ground surface are taken from infiltration rate data in DTN GS96090803212211.003 for present-day climates. The infiltration rate data from this TDIF are qualified. The infiltration rates at selected comparison locations in the repository block are 11.5 mm/year (center location) and 3.6 mm/year (edge location) for the preliminary base case nominal I property set and infiltration rate. The corresponding infiltration rates for the preliminary base-case nominal I times 5 property set are 57.5 mm/year (center location) and 18 mm/year (edge location). The repository coordinate location for the comparison is northing 233,400 m and easting 170,650 m for the center drift-scale model. The edge location is at northing 234,054 m and 171, 270 m. The differences in model formulations are now discussed.

In addition to the major differences related to model dimensionality and heat and mass flow conceptualizations applied to the host rock (for example, a conduction-only model), other smaller model differences include heat and fluid flow assumptions inside the emplacement drift. An additional major difference is in the implementation of waste packages located at the edge of the repository. The TH multiscale modeling and abstraction method uses explicit information from a three-dimensional mountain-scale model to include repository edge response to adjacent unheated mass. The PA testing models use abstracted data from a two-dimensional mountain-scale model to include repository-edge response to adjacent unheated rock mass. The waste-package response at repository-edge locations from the TH multiscale modeling and abstraction method is described in Section 3.5.1. The edge response for the testing model is described in the current section.

The heat transfer model (used in the testing models) applied in an open emplacement drift requires simplification because of the computational rigor of three-dimensional, TH drift-scale models. The two-dimensional LDTH and the three-dimensional DDT described in Section 3.5.1 implement an explicit model for radiation heat transfer from the heated surfaces. The additional connections resulting from radiant heat transfer do not hamper the numerical efficiency of the two-dimensional LDTH, and the three-dimensional DDT is a conduction-only model. Unfortunately, the same is not true for the three-dimensional drift-scale TH models. In order to reduce the numerical complexity of the model, a radiation heat transfer equivalence is implemented in the testing models only, using a simplifying thermal conduction mechanism. This method does not add any additional "non-diagonal" connections that must be solved by the numerical equation solvers used in the codes used to predict TH behavior at the scale of the drift. In addition to radiant heat transfer, assumptions are required when computing convective heat and mass transfer inside open drifts. The convective mode of heat transfer in an open drift is assumed to be a secondary mode. The relative importance of the assumption is compared to the dominant mode of heat transfer inside an open drift. An open drift is defined as an unbackfilled drift.

The "process-level" models for both abstraction and testing formulations were independently created. The abstraction methodology combines a series of one-, two-, and three-dimensional mountain-scale and drift-scale models both TH and conduction-only. It is computationally efficient and inherently contains waste-package variability, infiltration-rate variability, and

explicit edge-cooling responses. It is compared against a testing model that also contains waste-package variability, infiltration-rate variability, and abstracted edge-cooling responses. The TH abstraction methodology and process can be executed in a more efficient manner than the fully coupled three-dimensional TH drift-scale models. It is the job of the testing model formulations to increase confidence in the assumptions applied to the TH multiscale modeling and abstraction method. This testing procedure is important for both the VA models and eventually the TSPA-LA models.

3.6.1.1 Description of the Radiation Heat Transfer Assumption in the Three-Dimensional Thermal-Hydrologic Drift-Scale Testing Models

Drift-scale models (for example, the LDTH, DDT, and the testing models) contain detailed heat flow mechanisms from the waste packages to each other, floor, and drift walls. Inside an open drift, radiation heat transfer is expected to be the dominant mode of heat transfer. This is a very efficient mode of heat transfer. The incorporation of explicit radiant heat transfer in an open emplacement drift requires the modeler to compute (in advance) radiation configuration factors from the radiating surface (i.e., a waste package, invert floor, drift wall) to any other surface it can "see" and exchange energy with. The radiation configuration factor (also known as a view factor) represents the fraction of radiant energy emitted by surface *i* and intercepted by surface *j*. Receiving surfaces may include other waste packages, the ceiling, the floor, and the walls. One computational drawback of including explicit radiation heat transfer is the addition of radiation connections from a radiating surface to a distant receiving surface. Unlike conduction heat transfer, these connections add entries to the coefficient matrix that are progressively off the diagonal. That is, the coefficient matrix assembled when solving the conservation-of-energy equation begins to fill from the inside out. This fact will burden the equation solver during runtime. An additional consideration when including radiation connections in the drift model is an accurate accounting of all configuration factors that occur across the symmetry boundaries that are typically applied in three-dimensional drift-scale model analyses.

Since the three-dimensional drift-scale model is symmetric through the centerline of the drift and waste package (a lateral boundary condition), the radiation configuration factors are required for any modeled radiating surface that can view a surface through the symmetry boundary. This complication can be avoided with a conduction equivalent of a radiant heat transfer model. This assumption is applied in the PA testing models.

If one must duplicate the heat-transfer rate associated with radiation heat transfer using a different, less complex to implement heat flow mechanism, the best choice is conduction heat transfer. For radiant heat flow from a waste package to a large enclosure (the emplacement drift wall) completely surrounding the waste package, the rate of radiation heat transfer is:

$$Q_r = \varepsilon \sigma A \left(T_{WP}^4 - T_{DW}^4 \right) \tag{3-23}$$

where the view factor from the waste package to surrounding drift wall and invert is 1.0, ε is the emissivity of the waste package (= 0.8), A is the waste package area, $T_{waste\ package}$ and T_{DW} are the waste-package and drift-wall temperatures in (K), and σ is the Stefan-Boltzmann constant

(= 5.67 × 10^{-8} W/m^{2}K^4). The rate of heat transfer by radiation is equated to Fourier's law of heat conduction:

$$Q_c = k_{eq} A \frac{\Delta T}{\Delta x} \tag{3-24}$$

where k_{eq}, the equivalent thermal conductivity of the drift air element in the model, is the desired quantity. Equating the radiative heat transfer with the conductive heat transfer and solving for k_{eq} yields:

$$k_{eq} = \varepsilon\sigma\left(T_{WP}^2 + T_{DW}^2\right)\left(T_{WP} + T_{DW}\right)\Delta x \tag{3-25}$$

where Δx (≅ 2 meters) is an average distance from the waste package to the drift wall. This relationship for k_{eq} results in an approximation of radiant heat transfer using a thermal conduction equivalent. It is noted that the equivalent thermal conductivity depends on the waste-package and drift-wall temperature, consequently, it varies in time. In order to approximate the variability of k_{eq} in temperature (and hence time), Equation (3-25) is applied over a discrete range of temperatures in which the waste package and drift wall temperatures vary. Table 3-28 displays the results of k_{eq} over a discrete range of applicable temperatures for the drift-scale model simulations.

Note that the conduction equivalence used to approximate radiant heat transfer is three orders of magnitude greater than the standard thermal conductivity for air (= 0.03 W/m-K). The results of Table 3-28 are applied to the drift "air" elements found in the three-dimensional TH drift-scale testing models. They are open since the drift remains unbackfilled. It is noted that the temperature dependence in each of these ranges is very coarse. Additional values of k_{eq} would result as the applicable temperature ranges are made smaller and smaller. In the limit, Equation (3-25) can be evaluated at all temperatures as an explicit function of waste-package and drift-wall temperature during the drift-scale simulations. Using the simplified model shown in Table 3-28, a heat-transfer rate analogous to radiant heat transfer is included in the emplacement drift of the testing models. However, its driving mechanism is different than by explicit radiation.

Recall that radiant heat transfer is included **explicitly** in the drift-scale LDTH and DDT process models, making up the TH multiscale modeling and abstraction method. This is the model formulation that produced the base-case results for the TSPA-VA. Each of these process-level models contains simplifications in other respects (such as reduced dimensionality or conduction-only assumptions) so that explicit radiation can be included as the actual heat flow mechanism in an open drift. Furthermore, with the coupling of appropriate models and processes in the TH multiscale modeling and abstraction method, the simplifications that allow one to be able to apply explicit radiative heat transfer are completely addressed so that no physical processes are lost.

3.6.1.2 Description of the Convection Assumption in an Open Drift

It is necessary to show that the convective component of heat transfer in an open drift is not the main component of heat transfer. For a closed repository (forced convection is neglected), density gradients (occurring from the waste-package surface to the drift-wall surface) will result in fluid motion from the waste package to the drift wall. The fluid motion will transport heat from the surface of the waste package to the surface of the drift wall. It is assumed in the TH models that the relative contribution to the total heat transfer from the waste package surface (convection + radiation + conduction) via convection and conduction is much less than that of the radiative component. Consider conduction heat transfer through the air in an open drift. The conduction equivalent "radiation heat transfer" thermal conductivity is three orders of magnitude greater than the "stagnant" air thermal conductivity. Therefore, radiation heat transfer dominates conduction heat transfer in the open emplacement drift. Now let us consider natural-convection heat transfer.

The temperature difference between waste package and drift wall establishes a density difference within a gravitational field. This results in fluid motion inside the open drift. It is argued that the component of heat transfer from the waste package to the drift wall by natural convection (as a result of fluid motion) is much smaller than that by radiation heat transfer. A different "equivalent thermal conductivity" can also be computed for the fluid motion occurring within the drift between the hot-waste package and cooler drift wall (Incropera and DeWitt 1990; Kuehn and Goldstein 1976) based on experimentally derived correlation equations for concentric or eccentric cylindrical annuli. The equivalent thermal conductivity is made up of a sum of the conduction heat transfer through stagnant air and a component that accounts for the fluid motion. This equivalent "convection" conductivity is different than that previously defined for radiation as it is a function of the gas-phase Rayleigh and Prandtl numbers in an open emplacement drift. It is also a function of waste-package and emplacement-drift diameters. The Rayleigh number is a function of the fluid properties and indicates the ratio of buoyancy to viscous forces of the fluid phase in the drift. The Prandtl number is the ratio of the momentum diffusion to thermal diffusion. The equivalent thermal conductivity associated with the highest temperature range given in Table 3-28 and including a contribution for the fluid motion (based on natural convection only, not forced convection) is about 3.2 W/m-K. This is smaller than the 36 W/m-K associated with radiation heat transfer equivalent approximation for the same temperature range. For the lower temperature ranges given in the table, the difference in temperatures between the drift wall and waste package are slightly greater than at their peak values. This will result in the effective thermal conductivity that includes the fluid motion contribution that is slightly greater than 3.2 W/m-K. This is still less than the radiative component. The early time effect of a higher heat transfer rate by natural convection is short lived, since the peak temperatures difference between drift and waste package occur within the first 30 years after waste emplacement. For emplacement times after this peak, the density gradients within the open drift begin to approach zero.

Since this component of heat transfer (natural convection) is somewhat smaller than radiant heat transfer component, as shown above, the question of what value of bulk permeability should be assigned to the open drift elements in the drift-scale TH models needs to be addressed. For an open emplacement drift, the bulk permeability based on emplacement-drift geometry is given in Section 3.4.1 by Equation (3-1). However, this large-bulk permeability (approximately on the

order of square meters) causes numerical difficulties that do not allow the simulations to proceed at an acceptable time-step. It is necessary to reduce the bulk permeability of the drift elements in the models based on the ranges identified in the assumption section. This decision is justified based on the preceding argument of a relatively small contribution to the total heat transfer by the fluid motion (for example, heat transfer by natural convection). It is required, however, that the bulk permeability is not reduced so low that pressurization in the emplacement drift occurs. For bulk permeabilities in the darcy range or greater, pressurization in the medium will *not* occur as shown in Buscheck (1996). Additionally, since convective transport of heat is small, selection of a bulk permeability in the range of 5×10^{-12} m^2 to 1.0×10^{-8} m^2 does not alter the results of the near-field temperatures predicted by the drift-scale TH models.

3.6.1.3 The Scaling Method Applied to the Edge Models

Based on the idea that waste packages located near the edge of the repository behave as waste packages at the center of the repository, only at a lower thermal load, allows one to use a periodic model domain (like the drift-scale models) for other repository locations. This is a solution-matching technique using one-dimensional and two-dimensional mountain-scale models (Itamura and Ho 1998). This is an example of a model abstraction. This is justified by the idea that the flow of heat and mass in a drift-scale model far away from the emplacement drift is identical to that of a one-dimensional mountain-scale model. This implies that locally, the drift-scale model is three dimensional, but globally it is one dimensional. We compared two-dimensional results from a mountain-scale cross-section model to a set of one-dimensional runs (for a center column, west edge column and east edge column) using a series of lower AMLs. Our objective was to find a scaling factor, *f*, for the AML that provides the best agreement between two-dimensional mountain-scale model and lower AML one-dimensional mountain-scale runs with respect to temperature and air mass fraction of the drift elements. The scaling factors developed for the edge model and applied for testing purposes are given in Table 3-29. It is noted that the scaling factor for the center model is 1.0. That is, the reference AML for the center model is not scaled below the reference value of 85 MTU/acre.

The edge models (using periodic lateral boundary conditions) require a change in the AML as noted by the scaling factors given in Table 3-29. This is a direct result of the unheated rock masses on either bounding edge of the potential repository. The resulting early-time (0 to 1,000 years) edge model AML is reduced from 85 MTU/acre to 68 MTU/acre. After 1,000 years, heat losses from the edges are even greater. The late-time (1,000 to 100,000 years) scale factor is incorporated by scaling the heat output directly. The heat output itself is scaled, rather than an additional change in model AML, because there are complications associated with assigning a newly extended model domain the appropriate initial conditions (where the initial conditions occur as a restart at 1,000 years after waste emplacement). The late-time scaling factor is computed with respect to the early-time scale factor so that the heat output is scaled by 0.6/0.8 = 0.75. This is equivalent to a 51 MTU/acre repository AML. Therefore, lower AMLs are used to model waste package responses at repository edge locations.

3.6.1.4 Testing Model Results Compared to the TH Multiscale Modeling and Abstraction Method Results at Repository Center and Edge

The three-dimensional TH drift-scale (testing) models developed for repository center and edge locations are compared at the same locations to the results obtained from the TH multiscale modeling and abstraction method described in Section 3.5.1. The comparison is made for different waste package types located in the idealized drift segment. The range of waste packages compared include the coldest waste package in the model, the separate-disposal waste package; an average 21 PWR, and the hottest waste package, the design basis 21 PWR. The comparisons are made for the nominal I and five times nominal I preliminary base-case property sets and infiltration rates in order to consider a wide range of high infiltration rates. Recall, from Section 3.4.1, that the LDTH model in the TH multiscale modeling and abstraction method incorporates a dual-permeability modeling approach and the testing modeling incorporates a G-ECM approach. This governs fluid and heat flow in the mountain. In general, the G-ECM approach produces much flatter temperature profiles at the nominal boiling point (approximately 96°C at the local pressure at the repository horizon) for longer periods of time than does the dual-permeability modeling approach of the LDTH model.

From Figures 3-84 through 3-93 for the repository center comparison, it is noted that the TH multiscale modeling and abstraction method used to create the base-case results compares very well to the drift-scale model that includes waste-package variability coupled directly to the hydrology of the problem. (Recall that the DDT model is uncoupled from hydrology by using a conduction-only model. Indirect coupling for the TH multiscale modeling and abstraction method is then accomplished using a series of models and interpolation steps described in Section 3.5.4.) From Figures 3-84 through 3-88 for the present day (nominal) I property set (infiltration rate 11.5 mm/year), it is noted that the temperature comparison for the entire range of waste-package heat outputs is in excellent agreement for both of the model formulations. The initial heatup of the testing model is slightly slower than that of the TH multiscale modeling and abstraction method. This is most likely because there are differences in thermal-conductivity (of the host rock) relationships associated with the conduction-only and the TH models. Conduction-only models use a temperature approximation to provide an analogous "wet" and "dry" thermal conductivity. The temperatures peak at nearly the same value (about 200°C for the design-basis waste package) and at the same time (at about 25 years after waste emplacement). The relative-humidity predictions agree very well for the selected waste packages. Any early time differences in the relative humidities (refer to Figure 3-86) do not influence the waste package degradation models; therefore, these discrepancies are assumed to be inconsequential.

The comparison at higher infiltration rates (Figures 3-89 through 3-93) also indicates good agreement between the two model formulations. The multiscale modeling and abstraction method predicts slightly higher temperatures than the testing model. This may also be a result of conduction-only mountain-scale models (SMT model, see Section 3.5.1) not taking into account convection cooling processes driven by two different mechanisms. The first is by infiltrating water from the ground surface as it moves to the repository horizon. This may provide additional cooling as more water, introduced at about 19°C (the approximate temperature of the ground surface), moves from the ground surface to depth. This effect is included in the LDTH but not included in the SMT model. Both models are used to provide a temperature prediction. The second process is by convective cooling of the repository horizon by gas-phase currents.

The SMT model neglects the transport of heat away from the repository horizon in the form of buoyant convection fluid flow. From the figures it is noted that the discrepancy is mainly at early times and is much less, even at the higher infiltration rates (57.5 mm/year), after approximately 100 years after waste emplacement for the range of waste packages considered. The relative-humidity predictions are correlated to the temperature. The results for the higher infiltration rate are given in Figure 3-91 and Figure 3-93. These compare reasonably well.

The direct-disposal temperature and relative-humidity (Figure 3-94 and Figure 3-95) results compare model formulations at repository-edge locations. The comparison is in reasonably good agreement, though, not as good as repository center. The differences occurring in the formulations are most likely a result of the method in which the testing models are scaled for lower AML. In the testing models, it is assumed that waste packages at repository-edge locations behave as the center, only at a much lower thermal load. The TH multiscale modeling and abstraction method takes into account explicit heat dissipation into the unheated rock masses surrounding the repository periphery. Scaling of heat output at late times (for example, after 1,000 years as in the testing models) is not necessary since temperature dissipation is directly included by the SMT model as heat flows away from the repository into a large unheated region. Analogously, relative-humidity predictions agree reasonably well for both model formulations at repository-edge locations. In particular, it is noted that late-time relative-humidity behavior is in reasonably good agreement.

In summary, the TH multiscale modeling and abstraction method compares well to a testing model that directly includes waste-package variability coupled directly with the hydrology of the system. The testing model uses an abstracted approach to obtain waste-package response curves for repository-edge locations. Independently developed, the testing model formulation provides confidence that the TH multiscale modeling and abstraction method is representative of the TH processes occurring at Yucca Mountain as a result of emplacement of heat-generating wastes.

3.6.2 Model and Parameter Variation Approach

3.6.2.1 Additional TSPA-VA Property Sets

Three additional TSPA-VA property sets were used to capture uncertainties in the hydrologic properties. The preliminary base case was calibrated to widely varying infiltration rates. The DKM/Weeps property set was developed to allow more fracture flow to occur in the UZ, particularly in the non-welded geologic units. The TH property set was developed to better model the water imbibition rates in the rocks in and immediately below those that will host the potential repository. A complete description of the development of the "preliminary base case" and the DKM/Weeps property sets can be found in Section 2.6.1 in Chapter 2 of the TSPA-VA Technical Basis Document. A description of the development of the TH property set can be found in Section 3.5.2 and Section 3.6.2.2.

In the preliminary base-case property set, the van Genuchten fracture alpha was estimated using a calibration procedure. The property set was calibrated at the present-day infiltration, one-fifth of the present-day infiltration, and five times the present-day infiltration. The DTN for these three property sets are LB971100001254.001, LB971100001254.002, and LB971100001254.003 and the property sets are qualified.

In the DKM/Weeps property set, the variability is both in infiltration rate and in the fracture permeability. The fracture-matrix coupling strength, X_{fm}, was scaled globally to match matrix-saturation data. This property set allows an assessment of the effect of high fracture flow rates on the repository performance. The infiltration rates for which the DKM/Weeps property set was calibrated to were present-day infiltration, one-third of the present-day infiltration, and three times the present-day infiltration. The DTNs for these five DKM/Weeps property set are LB971212001254.006, LB971212001254.007, LB971212001254.008, LB971212001254.009, and LB971212001254.010, and these data are not qualified.

In the TH property set, the van Genuchten matrix alpha was increased in the TSw36 and TSw37. The van Genuchten fracture alpha was increased in the Tsw34, Tsw35, and TSw36 units, which allows the formation of a larger dryout zone and reduces the speed of the collapse of the dryout zone. This property set was calibrated only at the present-day infiltration rate. The DTN for this property set is LL980209004242.026, and it is qualified.

3.6.2.2 Thermal-Hydrologic Results of Additional TSPA-VA Property Sets

3.6.2.2.1 Mountain-Scale Results

The air mass fractions for the preliminary base-case property set (DTN LB971100001254.001, LB971100001254.002, and LB971100001254.003; these data are qualified) at both center and edge locations at both present-day and LTA infiltration rates can be found in Figures 3-96 through 3-99). The variability in the infiltration rate (one fifth to five times the nominal infiltration rate) for this property set was larger than that for any of the other property sets considered. The shapes of the air mass fraction curves were similar for the present day infiltration cases. The first minimum was lower for the higher infiltration case. For the long-term infiltration simulations, the highest infiltration case did not have the second air mass fraction minimum that was seen in all of the other preliminary base-case simulations.

The air mass fraction at the edge of the repository for the preliminary base-case property set simulations did not show much variability between infiltration rates. The curves for all but the highest LTA infiltration case were almost identical for all time. For the five-times-LTA simulation, the air mass fraction returned to near ambient conditions at around 1,000 years.

The gas flow rates for simulations using the preliminary base-case property set at both center and edge locations at both present-day and LTA infiltration rates can be found in Figures 3-100 through 3-103). At the center location, the gas flux peaks at 4×10^{-6} kg/m^{2}s at 20 years. Between 50 and 2,000 years, the gas-flow rates for the low-infiltration case were less than those from the higher-infiltration case. After 2,000 years, the three gas-flow rates for all three cases become similar with the gas-flow rate for the high-infiltration case being slightly lower than those from the other two cases. For the climate change simulations, the curves for one fifth and the nominal LTA are similar in shape to those at present day conditions. For the five-times-LTA infiltration-rate case, the gas flux returned to near ambient conditions after 2,000 years.

At the edge of the repository, there was not much difference between gas-flux rates generated by the different property sets at either present day or at the LTA infiltration conditions. Except for

the five-times-LTA case, the gas phase fluxes at the center of the repository were either similar or slightly lower than those at the edge of the repository.

The air mass fractions for the DKM/Weeps property set (DTN LB971212001254.006, LB971212001254.007, LB971212001254.008, LB971212001254.009, and LB971212001254.010; these data are not qualified) at both center and edge locations at both present-day and LTA infiltration rates can be found in Figures 3-104 through Figure 3-107). At the center of the repository, the air mass fractions vary considerably depending upon the fracture permeability. When the fracture permeability was high, the air mass fractions did not ever decrease below 10^{-3}. The air mass fractions were almost the same despite the infiltration rates being one third and three times the present-day infiltration rates. For the DKM/Weeps case at the mean fracture permeability and at the present-day infiltration rate, the air mass fraction curve is similar to the base-case property set results with two minima. For the DKM/Weeps cases with a minimum fracture permeability and at one third and three times the present day infiltration rates, the air mass fraction dropped below 10^{-7} after 25 years and did not rise above 10^{-7} until after 1,000 years. Similar trends were seen in the climate change infiltration simulations.

At the edge of the repository, the air mass fraction time-history curves were much more strongly dependent upon the selection of the fracture permeability than on the infiltration rate. For the two cases with the maximum fracture permeability, the air mass fraction reached a minimum of 0.02. The air mass fraction dropped below 10^{-3} for 20 years at the mean value of the fracture permeability, and the air mass fraction dropped below 10^{-3} between 15 and 500 years for the minimum value of the fracture permeability. Similar trends were seen in the climate change infiltration simulations.

As in the case for the base-case property set simulations, the air mass fraction is still very strongly dependent upon the location in the repository (center vs. edge). When the fracture permeabilities are high, the difference between the air mass fractions time-histories at the center and the edge was always small. The air mass fraction at the center was almost always less than one order of magnitude smaller than that at the edge of the repository. For the other DKM/Weeps simulations (Kf-minimum and Kf-mean), the differences in the air mass fraction time-histories from center to edge were much larger.

The gas-phase flux plots for the DKM/Weeps property set simulations are presented in Figures 3-108 through 3-111. At the center of the repository, the gas flux for all of the DKM/Weeps property set simulations peaked at 4×10^{-6} kg/m^{2}s between 10 to 20 years after waste emplacement. The low infiltration rate with the minimum fracture permeability case had a lower gas-flow rate than the other cases between 30 and 1,000 years but the effect on performance should be almost the same as the high-infiltration rate with the minimum fracture permeability case because the air mass fractions for those two simulations were less than 10^{-7} during that period. After 2,000 years, the gas fluxes have separated, revealing some trends. The stronger of the two trends is that the gas fluxes were higher for the cases with the higher fracture permeability than those using a lower fracture permeability. The weaker of the two trends is that the gas-flow rates, for cases with the same fracture permeability, are higher when the infiltration rates are lower. For the LTA infiltration rate simulations, the effects of the variability of infiltration rate and that of the fracture permeability were the same on the magnitude of the gas flux after 2,000 years.

At the edge of the repository, the gas fluxes all peaked near 3×10^{-5} kg/m^{2}s at 20 years. The gas-flux curves were almost the same for the first 1,000 years, but the effects of the variable infiltration rate and variable fracture permeability were seen after 2,000 years. The gas flows were higher when the fracture permeabilities were large and the infiltration rates were small. As was the case at the center of the repository, the variability in the fracture permeability had a greater effect on the gas-flow rates than did the variability in infiltration rate. At the LTA infiltration rate, the effect of the variability of the infiltration rate was more important than it was during the present-day infiltration case, but the effect was still smaller than the effect of the variability of the fracture permeability.

The air mass fractions for the center and edge locations using the TH property set (DTN LL980209004242.026; these data are qualified) at both present-day and LTA infiltration rates are presented in Figure 3-112. The air mass fraction at the center of the repository follows the same two minimum patterns at around 50 and 500 years that were seen in other simulations. The air mass fraction at the edge of the repository has one minimum at 30 years. The variability in air mass fraction is a much stronger function of repository location than it is of the infiltration rate for this property set.

The gas flux time-histories for the center and edge locations using the TH property set at both present-day and LTA infiltration rates are presented in Figure 3-113. For most of the 100,000-year simulation, the gas flux for the LTA infiltration rate was lower than that for the present-day infiltration rate. The difference between center and edge locations was larger than the differences resulting from the variation in infiltration rates.

The air mass fraction and gas-flow rates at center and edge locations and at present-day nominal I infiltration rate for the base case, the preliminary base case, DKM/Weeps, and the TH property set are presented in Figures 3-114 through 3-117. All of the curves match up quite well with each other. At this infiltration rate, the air mass fractions and the gas-flow rates are a strong function of location (center vs. edge).

3.6.2.2.2 Drift-Scale Results

The results for the engineered-barrier response curves at the waste-package surface were given in Section 3.5.5 for the base-case properties, thermal and hydrologic, and reference-repository design. Engineered-barrier response curves include waste-package surface temperature and relative humidity. Other TSPA property sets were created in order to bound the potential range of unsaturated flow uncertainty. The results for the engineered barrier response curves from the preliminary base case, TH, and DKM/Weeps hydrologic property sets are also applied to the reference-repository design. The results for the preliminary base case and the TH property sets are obtained from the TH multiscale modeling and abstraction method. The results for the DKM/Weeps hydrologic property set are obtained from the PA testing drift-scale models. All of the simulated results are computed as if the LTA climate state is in effect for all times after waste emplacement. All of the hydrologic property sets are given in Chapter 2 of the TSPA-VA Technical Basis Document.

Preliminary Base Case

Figure 3-118 displays the repository subregional variability for each of the six regions. The results are analogous to the results given in Section 3.5.5 for the base case, as one would expect. For the LTA climate, the averaged maximum temperatures are about 160°C. The extended time spent at the nominal boiling point for this property set is less than the time shown for the base-case results. This is mainly a result of reduced capillarity in fractures for the base-case property set since the infiltration rates are the same. The extent and duration of superheated conditions predicted by the preliminary base-case properties, at the waste packages, is less than the base case. This results in lower temperatures and higher relative humidities at earlier times after waste emplacement.

Figure 3-119 and Figure 3-120 display waste-package variability (temperature and relative humidity) for the NE subregion and the maximum potential variability in average waste package surface temperature in the NE subregion for preliminary base-case properties and associated infiltration-rate uncertainty for the LTA climate. From the figures it is clear that the infiltration rate uncertainty drives the TH response at the repository horizon by greatly reducing temperatures at high percolation rates.

Figure 3-121 displays the property set variability for the NE subregion for all four property sets considered in the TSPA-VA. This is representative of the LTA climate. It is noted that the DKM/Weeps result shown in this figure is a result of the TH multiscale modeling and abstraction method.

Thermal-Hydrologic Property Set

The TH property set is a hydrologic property set with reduced capillarity in the fractures and matrix around and in the repository host units. In attempting to model the SHT and the LBT with the hydrological data for the tsw36 (Tptpln) unit, it was found that capillary forces associated with these property values in the repository host rock were too strong, contrary to experimental data, to allow the formation of a superheated dryout zone (Hardin 1998). This difficulty was attributed to large values of matrix imbibition diffusivity D_{imb} in that unit, which led to rapid rewetting of the rock.

This difficulty was partially overcome in November 1997 by the development of a TH parameter set calibrated by Lawrence Livermore National Laboratory (LLNL) and Lawrence Berkeley National Laboratory (LBNL) with temperature measurements from the SHT. Analysis of the SHT in Hardin (1998, pp.3-22 through 3-28), shows that the value of D_{imb} for the tsw36 in the preliminary base-case property set is too large to allow rock dryout and temperature rise in the nominally superheated zone. The reduced value of D_{imb} for the tsw36 produces more rock dryout in this unit and a closer match to temperatures observed in the SHT. These parameters are summarized in Table 3-30 and Table 3-31, respectively, for the matrix and fractures.

The parameter set actually used for the sensitivity studies was developed at LLNL by modifying the initial TH set. Table 3-32 contains the matrix parameters in the tsw36 and tsw37 units for this modified TH property set. The TH property set used for the sensitivity studies in the TSPA-VA contains data tracking information found in DTN LL980209004242.026. Fracture

properties, and matrix properties for other units, were not changed from values in the TH set. The modifications were made so that the value of D_{imb} for the tsw36 and tsw37 units are the same as those in the tsw34 unit. These changes were made because laboratory measurements from Flint et al. (1996b, taken from Table 2) indicate that the values of D_{imb} for the tsw36 and tsw37 units are no greater than those for the tsw34 unit. The principal change was a reduction, by a factor of 28, in the value of D_{imb} for the basal vitrophyre (tsw37). The value for the tsw36 unit was reduced by a factor of 2.8. Model calculations with these parameters indicate more rock dryout in both of these units than was obtained with the TH set.

Figure 3-122 and Figure 3-123 indicate the average waste-package temperature for each of the six repository subregions and the waste-package temperature and relative-humidity variability in subregion NE, respectively. From these figures and earlier preliminary base case figures, it is evident that the imbibition potential of the fractures and matrix influence the response curves at the waste-package surface. The reduced matrix imbibition diffusivity (which reduces the rate of rewetting) has increased temperatures at their peak values as well as slightly extended the boiling period during repository cooldown. The differences between this property set and the base-case property set, however, is not very large. A discussion of this TH uncertainty, in the form of an additional property set, as applied to dose rate is given in Section 3.7.

Dual Permeability Model/Weeps Property Set

Description of Property Set - The primary goal of the DKM/Weeps hydrologic property set is to model the hydrology of the natural environment as a fracture-dominated flow system. In Section 2.6.1 in Chapter 2 of the TSPA-VA Technical Basis Document, Unsaturated Zone Sensitivity Studies, an overview of the DKM/Weeps property set conceptualization is presented.

Converting the DKM/Weeps Property Set from DKM to G-ECM - A description of the DKM, ECM and G-ECM conceptual flow models is contained in Section 3.4.2 In order to examine the effects of the DKM/Weeps alternative property set on the TH response of the waste package environment, a G-ECM assumption was made so that the analysis could be performed using the testing models developed by PA. For a measure of completeness, the DKM/Weeps mean fracture permeability (K_f) case was also applied in the TH multiscale modeling and abstraction method.

In the DKM/Weeps concept, water primarily flows in the fractures. The DKM modeling approach necessary to attain this flow response specifies a reduction in fracture-matrix conductance which greatly inhibits imbibition of water from the fractures into the matrix elements. The matrix satiation control of the G-ECM conceptual model was used to create an approximation to the Weeps fracture-dominated flow system. In each of the ambient DKM simulations used to compute the steady states values for the DKM/Weeps property sets, the resulting steady state matrix saturation for each stratigraphic rocks unit is preserved for use in the approximate G-ECM model. Therefore, once the matrix elements reach the saturation threshold derived from the ambient DKM models, the flow in the fractures initiates.

Model Matrix Simulated - Five DKM/Weeps parameter sets are described in Section 2.6 in Chapter 2 of the TSPA-VA Technical Basis Document, Unsaturated Zone Sensitivity Studies. The same five calibrated parameter sets were examined for their TH performance in this section.

The five property sets are: (1) maximum fracture permeability calibrated to three times the present-day surface infiltration, (2) maximum fracture permeability calibrated to one-third the present-day surface infiltration, (3) mean fracture permeability calibrated to the present-day mean surface infiltration, (4) minimum fracture permeability calibrated to three times the present-day surface infiltration, and (5) minimum fracture permeability calibrated to one-third the present-day surface infiltration. All five property sets were simulated twice, first with the current infiltration rate and then again with an increased surface infiltration rate that approximated the LTA climate state.

Comparisons of Property Set Extremes – Of the modeled property sets there are two bounding extreme sets. The minimum fracture permeability set with the one-third-present-day infiltration will produce the weakest of all the DKM/Weeps flow systems simulated. The strongest Weeps flow system will be produced by the maximum fracture permeability with the three-times-LTA infiltration parameter set. Figures 3-124 through 3-126 show the variability in the waste package temperature and relative humidity for the average 21 PWR, the design basis 21 PWR, and the separate (direct-) disposal waste package using the DKM/Weeps property set.

Figure 3-124 shows the average CSNF waste package surface temperature and relative-humidity response curves for the bounding DKM/Weeps property sets. The low fracture-permeability response is very similar to the mean fracture-permeability set after the waste package surface temperature falls below 100 degrees. Both the low- and mean-permeability curves remains at the boiling threshold from 1,300 years out to approximately 6,000 years of emplacement. The high fracture-permeability set response curve falls quickly to the boiling threshold after approximately 200 years and remains at the threshold until approximately year 1,300th. The relative-humidity response curves for all three of the property sets show that the waste packages are well into the aqueous-corrosion regime (i.e., >85% relative humidity) by the time they fall to boiling and sub-boiling temperatures.

Figure 3-125 shows the design-basis CSNF waste package response curves. Though the design-basis waste packages are by definition the hottest packages allowed into the repository, their response curves after approximately 500 years are virtually identical temperature wise to the average 21 PWR waste-package curve, and the relative-humidity response curves are extraordinarily similar as well. The main difference between the average packages and the design-basis packages appears to be the peak above boiling temperatures. Since no temperature thresholds are broken and corrosion is not initiated in this regime, there should be very similar waste packages performance reported between the average SNF and design-basis SNF.

Figure 3-126 shows the separate disposal waste package surface temperature and relative-humidity response curves. As with the design-basis waste packages, the only differences observed with the temperature-response curves appear to be with the above boiling temperatures; after 1,300 years the response curves are identical. Between year 500 and year 1,300, the mean fracture permeability response appears to border on the boiling zone more closely than with the SNF packages, but other than this, performance should match closely with the SNF package performance.

Comparisons of LTA Response Curves -In order to conservatively judge the responses of the waste packages to the DKM/Weeps conceptual model, Figures 3-127 through 3-129 show all of the high-flux, LTA, scenarios.

Figure 3-127 illustrates the response curves of the average CSNF waste packages for all five DKM/Weeps hydrologic parameter sets in the LTA climate state. It is noted from this figure that the waste-package surface response temperatures are basically independent of rock property set when the waste package surface cools to the nominal boiling point, the controlling parameter is the infiltration rate. This is indicated in the figure by the convergence of the maximum and minimum fracture permeability with LTA infiltration multiplied by three curves at late times. The maximum and minimum fracture permeability with LTA infiltration divided by three curves similarly converge at late times. Early time behavior is also influenced by the infiltration rate ($T_{I/3} > T_I > T_{I*3}$, where T is temperature), however, the intrinsic fracture properties also influence the movement of heat generated condensate away from the dryout zone. This difference in water vapor generation and transport and subsequent condensation at the fringe of the dryout zone may result in the separation of the temperature curves at early heating times. The packages begin to fall from above-boiling temperatures into the boiling threshold region between 300 and 800 years. The high-infiltration LTA models are the first to fall into sub-boiling temperatures after 1,300 years of emplacement. The current infiltration model, with the LTA climate conditions imposed, falls below boiling just after 2,000 years. And the low-infiltration LTA models proceed into sub-boiling temperatures after 4,000 years of emplacement.

Comparisons of Current Climate versus LTA Climate Conditions - The base-case DKM/Weeps property set, when shown with the base-case DKM/Weeps set with LTA climate conditions imposed, should be the most realistic responses to expect from a fracture-flow-dominated system.

Figure 3-130 shows the temperature and relative-humidity response curves of the average SNF waste packages when simulating with the mean fracture permeability and mean infiltration rate, with and without the LTA climate condition imposed.

The temperature response falls from the above boiling state into the boiling region after 900 years under the current climate conditions and after 300 years with the LTA conditions. The temperatures remain at the boiling threshold for 4,000 years for the current-climate model and for 2,200 years for the LTA model.

Figure 3-131 shows the temperature and relative-humidity response curves of the design basis CSNF waste packages in the mean DKM/Weeps property set model, both with and without LTA conditions imposed. Because peak temperatures are higher, the surface temperatures do not fall into the boiling threshold region until 1,000 years for the current-climate model and 550 years for the LTA model. Once the package surface temperature falls into the boiling threshold region, the response curves converge with those of the average SNF package and behave identically throughout the rest of the simulation.

Figure 3-132 shows the temperature and relative humidity response curves of the separate disposal waste package. The package barely breaks into the above boiling regime before the surface temperature decays back into the boiling threshold region after 700 years for the current-

climate case and just 100 years for the LTA case. Because of the internally generated decay heat and the absorption of decay heat from neighboring SNF packages the package is able to remain in the boiling threshold region until it too converges to virtually the identical temperature response curve as the average SNF package.

All of the packages in the simulated drift converge to virtually identical response curves after 1,000 years of emplacement. Once the temperature falls into sub-boiling temperatures the relative humidity is high enough to initiate aqueous corrosion conditions.

Comparisons of Model Results with TSPA-VA Thermal-Hydrology Modeling and Abstraction Method Results - A mean fracture permeability with current-climate conditions DKM/Weeps scenario was simulated using the TH multiscale modeling and abstraction method. Figure 3-74 and Figure 3-121 show the TH multiscale modeling and abstraction method results. Comparing Figure 3-74 and Figure 3-121 with Figure 3-130 of this section, we can analyze the similarities and differences. The most notable difference between the response curves is the presence of a temperature plateau in the drift-scale model (Figure 3-130), that is not present in the TH multiscale modeling and abstraction method. This can be attributed to the difference in conceptual models used by each model and to the limiting dimensions of the drift-scale model. The TH multiscale modeling and abstraction method was able to simulate the base-case DKM/Weeps property set with a DKM conceptual model; it took a great deal of computational time but the results were achieved. Because of the dual continuum basis of the DKM model and the dimensional difficulties taken care of in the TH multiscale modeling and abstraction method, the removal of heat and water through fracture pathways is so efficient that the temperature curve passes directly through the boiling threshold point as it cools down. The next interesting difference between the model results is the consistently lower temperatures predicted by the TH multiscale modeling and abstraction method when compared to the drift-scale model. This, once again, is the result of the model conceptualization. The drift-scale model simulates a discrete section of only seven waste packages and uses the G-ECM approximation of the DKM/Weeps parameter set. The TH multiscale modeling and abstraction method is able to account for full three-dimensional mountain-scale removal of heat and it can simulate the DKM model when using the DKM/Weeps property set. So even in time frames which do not include the effects of latent heat return and boiling, it is expected that the drift-scale model will produce results that are hotter.

Conclusions Regarding In-Drift Sensitivity to DKM/Weeps Property Sets

There is very low sensitivity between the thermal response of the waste package and the variation of DKM/Weeps parameter sets. This was exemplified best by the comparisons contained in Figures 3-127 through 3-129, where it was shown that after 200 years the results were nearly completely independent of the range in fracture premeability considered and heavily dependent on infiltration rate.

It was observed that, with the package spacing needed to achieve an 85 MTU/acre drift loading and the attributes of the flow system developed by the DKM/Weeps property set, each of the waste-package types would converge to the same temperature and relative-humidity response. The convergence of response curves by the many different types of packages in each simulation

happened at individual times after emplacement, but it always occurred while the package was still in the boiling threshold region.

Imposing the LTA climate conditions on any of the DKM/Weeps scenarios will cool the temperature response curve by as much as ten degrees from the current-climate case. The application of the LTA climate condition always directly and consistently affects the temperature-response curve.

Assessment of Rock Dryout Surrounding Drifts

The waste decay heat generated in the emplacement drifts is expected to raise the temperature in the surrounding rock well above liquid water boiling temperatures. As the liquid-water in the nearby tuff boils, areas of zero saturation develop around the emplacement drifts. The areas around the emplacement drifts that have liquid saturations of zero are referred to as the dryout zones.

For PA purposes the interest lies in the extent and duration of these dryout zones. Indeed, if the dryout zones of neighboring drifts merge together then a complete repository-scale condensation cap may form. Some of the heat displaced water may drain between drifts by gravity in the fracture system. This "condensate drainage" process occurs early as the dryout begins to extend across the drifts. For remaining water above the drifts a repository-scale condensation cap can potentially divert large volumes of water to the edges of the repository, preventing water from dripping into the drifts and keeping lower relative humidities in the drifts. However, it is noted that this model analyses applies a G-ECM conceptual flow model. While this flow model allows increased fracture flow at matrix saturations near ambient (or what would be above in the case of a condensate zone), condensate drainage through a zone of rock below ambient (as in a dryout zone) is governed by capillary pressure equilibrium such that fracture flow is redirected into the matrix. Re-evaporation occurs in the matrix and the process continues. A nonequilibrium flow model between fractures and matrix rock may preclude this behavior and with this, the development of a repository wide condensate zone above the drifts.

Alternatively, if the dryout zones from drift-to-drift do not merge to form a continuous repository-scale condensation cap, performance of the repository would still be enhanced by dryout zones that extend only around the emplacement drifts themselves. Though a drift-scale condensation cap, would not be as effective in diverting water as a repository-scale condensation cap it would still produce many of the same performance attributes. Any amount of dryout around the drifts will decrease the likelihood of water drips in the drifts and keep relative humidities low at the waste-packages' surfaces. However, this benefit is realized only as long as the temperatures at the drift wall remain above boiling.

For the purposes of examining the dryout zones around the emplacement drifts we will use a version of the TSPA-VA rock property set referred to as the DKM/Weeps property set. This property set bounds the base-case property set by varying fracture permeability. Five separate property sets were used to analyze and bound the possible dryout zone development: (1) maximum fracture permeability calibrated to three times the present-day surface infiltration, (2) maximum fracture permeability calibrated to one-third the present-day surface infiltration; (3) mean fracture permeability calibrated to the present-day surface infiltration; (4) minimum

fracture permeability calibrated to three times the present-day surface infiltration; and (5) minimum fracture permeability calibrated to one-third the present-day surface infiltration. All five property sets were simulated four times, a center and an edge model with the current infiltration rate and then the center and edge model again with the increased surface infiltration rate that approximates the LTA climate changes.

Dryout Zones Near Center Region of the Repository

K_f max, three times nominal infiltration, current-climate and LTA climate conditions

Dryout zones formed around the modeled emplacement drifts are very small to nonexistent. Relatively cooler defense waste packages do not create enough energy to even start a zone of dryout in the surrounding tuff. The hotter design-basis SNF waste packages can produce only short-lived dryout pockets that peak after 35 years, with dryout zones only about four meters in depth. In the current-climate model, what little dryout does occur around the emplacement drift has broken down to sporadic pockets of dryout after 700 years. After 1,500 years of emplacement, all of the surrounding tuff has begun to re-saturate.

In the LTA climate model even less dryout is observed and what very little dryout there is begins to break down after 70 years. After 300 years, all of the surrounding tuff elements are observed to have started re-saturating.

K_f max, one-third nominal infiltration, current-climate and LTA conditions

Under the one-third nominal infiltration climate conditions the dryout region surrounding the emplacement drifts is observed to unsteadily expand for 500 years. Dryout zones from neighboring drifts have partially merged to form an incomplete condensation cap before a gradual recession. After 4,000 years the dryout cap surrounding each emplacement drift begins to break down leaving intermittent dryout zones. Finally, all of the tuff elements surrounding the drifts begin re-saturating after approximately 6,000 years of emplacement.

Under the LTA climate assumption the breakdown of the drift-scale condensation cap is observed to occur after 1,600 years, and the last of the sporadic dryout zones collapses after 3,500 years of emplacement.

K_f mean, nominal infiltration rate, current-climate and LTA conditions

In the current-climate model, a dryout zone forms around the drift and steadily increases into the surrounding rock for 50 years. Unfortunately, a merging of the dryout zones between neighboring drifts was not observed so a full repository-level condensation cap did not occur. The dryout zones begin to gradually shrink after their peak at 50 years of emplacement and then disappear completely after approximately 5,000 years.

As expected with the LTA adjusted model, the increase in infiltration flux removes considerably more thermal energy from the emplacement drifts than the current-climate model. The extent of the dryout zone is thus greatly reduced, with the maximum extent of the dryout zone being reached after 40 years. The dryout zone surrounding the emplacement drifts begins to break

down after 600 years, and completely shrinks back to the walls of the emplacement drift after only 1,800 years.

K_f min, three times nominal infiltration, current-climate and LTA conditions

In the three-times-nominal infiltration model the expansion of the surrounding dryout zones is very limited. Merging of neighboring dryout zones is not observed and the first breakthrough of the drift-scale condensation cap occurs after only 350 years of emplacement. All areas of dryout are observed to disappear after 1,200 years.

The LTA climate conditions overwhelm the tuff surrounding the emplacement drifts causing the dryout zone to break down after just 60 years of emplacement. The last of the de-saturated elements begins re-saturating after just 230 years.

K_f min, one-third-nominal infiltration, current-climate and LTA conditions

For the current-climate model, the lower infiltration rate and minimum fracture permeability produced a complete dryout zone that was more stable than any other observed using the other hydrologic property sets. After only 30 years the dryout zones formed around the drifts begin to merge with the dryout zones of neighboring drifts. After 150 years the dryout zone has spread to a point where it forms a complete or repository level condensation cap above the drift. The dryout zone continues to expand for the first 700 years of emplacement. The drift-to-drift dryout zone connection is broken after 1,000 years, but the drift-level condensation cap continues. The dryout zones around the drifts are not observed to completely vanish until after 5,000 years of emplacement.

When LTA conditions are imposed on the model, the observed dryout zones are not as complete or stable as with the current-climate model. The dryout zone around the emplacement drifts advances relatively quickly but peaks after only 50 years. The merging of neighboring drifts' dryout zones does not completely occur even at the peak. The dryout zone around the drifts gradually recedes after 70 years and after 500 years there are only pocketed regions of dryout remaining. After 1,500 years there are no dryout zones surrounding the drifts.

Dryout Zones Near Edge Regions of the Repository

As described in Section 3.2, the drift-scale edge model is a scaled version of the drift-scale center model. Note that the scalings that were added to the edge model in order to achieve the cooler temperatures that are expected near the edge of the repository could impact the formation of dryout zones both positively and negatively.

K_f max, three-times-nominal infiltration, current-climate and LTA climate conditions

The current-climate-conditions model developed dryout zones that were limited in extent and unstable in nature. The dryout zones that are observed to form around the emplacement drifts form a complete drift-scale condensation cap but never extend far enough to merge with the neighboring drifts' dryout zones. The dryout zones surrounding the drifts go through a great number of perturbations during their existence and have collapsed to intermittent dryout areas

after only 1,000 years of emplacement. After 1,600 years of emplacement, even the small pockets of dryout around the drifts have disappeared completely.

Once the LTA multiplier is used on the already high infiltration rate, the tuff surrounding the emplacement drifts is completely overwhelmed by the liquid flux. Only a few pockets of dryout appear around the emplacement drifts near the hotter waste packages. What few pockets of dryout do appear are short lived and very limited in extent. The pockets of dryout that are observed begin recessing after 50 years and are non-existent after 500 years of emplacement.

K_f max, one-third-nominal infiltration, current-climate and LTA conditions

Using the current-climate conditions, the dryout of the surrounding tuff is slow and unsteady. After 300 years of emplacement, the dryout zones from neighboring drifts begin to merge, but even after 500 years of emplacement, when the dryout zones begin to recess, a complete repository-level condensation cap is not achieved. After 1,000 years of emplacement the dryout zones have recessed to where there is no longer any communication between dryout zones of neighboring drifts. The breakdown of the drift-scale condensation cap occurs after 1,600 years and after 1,800 years the last of the "dry" elements begins to re-saturate.

The LTA climate model behaves similarly to the present day I/3 climate. The breakdown of the dryout zone encompassing the emplacement drift occurs after 1,100 years, and approximately 200 years later all traces of dryout have disappeared.

K_f mean, nominal-infiltration-rate case, current-climate and LTA conditions

The edge effects (edge cooling processes) inherent in this model prevent the dryout zone from extending as far as it does in the center region. The maximum extent of the dryout zone is gradually reached after 600 years as the percolation flux is diverted around the zone. Formation of a repository-level condensation cap does not occur, but the dryout zones about each of the emplacement drifts are complete and substantial. The dryout zone formed about each drift gradually shrinks until it is essentially gone after 1,800 years.

In the LTA case, the maximum extent of the dryout zone occurs after only 90 years and is not as expansive as the current-climate case. The dryout zone that is formed breaks down after 800 years of emplacement and essentially disappears after 1,400 years.

K_f min, three-times-nominal infiltration, current-climate and LTA conditions

The current-climate model develops a dryout zone that stops expanding after only 50 years of emplacement. The dryout zone steadily recedes after 70 years until the first breakthrough of the drift-scale condensation cap occurs after approximately 700 years of emplacement. After 1,600 years of simulation there is no observable dryout zone present.

The elements surrounding the drifts in the LTA model are quickly overcome by the massive infiltration flux imposed on the model. The dryout zone that does form begins collapsing back to the drift walls after 110 years. Remarkably, traces of the drift dryout zones are visible until approximately 500 years.

K_f min, one-third-nominal infiltration, current-climate and LTA conditions

As in the center model, the lowering of both the infiltration rate and the fracture permeability leads to a larger expansion of the dryout zone about each drift. After 60 years, the dryout zones of neighboring drifts begin to merge. After 350 years, the dryout zones have spread to a point where they form a complete repository-level condensation cap above the drifts. The growth of the dryout zone continues after the formation of the repository-scale condensation cap and does not begin to recede until after 700 years of emplacement. The breakthrough of the repository-level condensation cap occurs after 1,100 years of emplacement, and all communication between neighboring drifts' dryout zones disappears after 1,300 years. The dryout zones gradually recede until breakthroughs to the drift walls begin occurring after 1,800 years of emplacement, and then they are completely gone after 2,500 years.

With the LTA climate assumption imposed, a limited extent of dryout surrounding the emplacement drift is observed. A complete drift-scale condensation cap is formed along the emplacement drifts but the dryout zones never merge with neighboring drift dryout zones. The drift-scale condensation cap breaks down after 800 years of emplacement, leaving only intermittent areas of the emplacement drifts covered by limited dryout zones. All of the surrounding tuff is beginning to regain some level of saturation after 1,100 years.

Conclusions Regarding Dryout Zone Formation

Adjusting the modeled fracture permeability in order to bound the predicted response of the near-field environment shows the relatively low sensitivity of the system to that parameter. The dominant parameter controlling the extent of tuff dryout was the infiltration rate. The Table 3-33 summarizes the discussed results by displaying the observed dryout duration times. While Table 3-33 makes the relationship between infiltration rate and drift dryout fairly apparent it does not make a relationship between fracture permeability and drift dryout as apparent. The fact that the center and edge models that used the low infiltration rate and the minimum fracture permeability were the only ones to form repository-level condensation caps is easily over shadowed by the longer dryout duration times observed in many of the maximum fracture permeability models.

The results of the base-case mean DKM/Weeps TH properties show that a repository-scale condensation cap is unlikely to form. A substantial dryout zone is predicted to form that should reduce the likelihood of drips into the drift for 1,800 to 5,000 years, depending on the nearness of the emplacement section to the edge of the repository. The conservative assumption of increasing the infiltration to the LTA reduces the predicted "no drip" period to a range of 1,400 to 1,800 years, once again depending on the relative location to the edge of the repository.

3.6.3 Alternative Repository-Design Options

Enhanced repository designs include use of backfill and drip shields either directly on the waste packages or on top of the backfill material. Additional options include ceramic coatings on the waste packages. These options are expected to reduce the amount of liquid water in contact with the waste package. The presence of backfill also reduces relative humidity for a longer period of time after waste emplacement. A backfilled repository design option is considered, using the

reference repository point-load design. The backfill materials considered for repository emplacement are quartz sand and crushed tuff. Backfill is emplaced in the drift 100 years after initial waste emplacement. It is assumed that the backfill material is emplaced "essentially dry" and that the backfill material only partially fills the emplacement drift.

Where backfill partially fills the drift, thermal radiation is important in the cavity between the surface of the backfill and the drift crown. The invert material represents about 11% of the emplacement-drift area, the air cavity above the backfill and below the crown of the drift represents about 13%, while the remaining space is filled with backfill and the waste package itself. Thermal radiation is incorporated in models with discrete heat sources (e.g., the DDT model). Drift-scale model calculations were conducted for cases without backfill and for cases in which an engineered backfill is emplaced at 100 years.

For drift-backfill scenarios, the open space in the drift is filled with a uniform, porous material. The grid for the model with backfill has more resolution in the drift than the model with no backfill in order to better represent the influence of seepage and capillary-driven wicking in the backfill.

The crushed-tuff backfill is represented using the DKM–so that disequilibrium processes are allowed between the intragranular porosity (represented by the matrix continuum in the DKM) and the intergranular porosity (represented by the fracture continuum in the DKM). The crushed-tuff backfill assumes that the intragranular porosity consists of 3.2-mm-size grains and the tsw35 matrix property values from the TSPA-VA base-case hydrological property set. Because grain-to-grain liquid-phase flow only occurs at the points of contact between crushed-tuff grains, the matrix-to-matrix connectivity factor is assumed to be 0.001, thus representing the highly tortuous manner in which grain-to-grain flow will occur. The intergranular porosity of the crushed-tuff matrix has a bulk permeability of 100 darcy and capillary properties that are representative of gravel. Rewetting of the backfill can occur from seepage and capillary-driven wicking in the intragranular and intergranular porosity. For both the crushed-tuff backfill and the quartz-sand backfill, the thermal conductivity of the backfill is assumed to be 0.67 W/m-K and backfill is assumed to be emplaced at 100 years.

For the quartz-sand, the intragranular porosity is assumed to be nonporous and impermeable; hence, it functions like a single continuum. Because a DKM is used, the matrix and fracture continuums both represent the intergranular porosity, which has properties that are typical for a well-sorted, medium-to-coarse sand. The hydrological properties of the sand are abstracted from. (Personal communication with Ken Lee, Lawrence Livermore National Laboratory, for backfill properties. 1998). Rewetting of the backfill can occur from seepage and capillary-driven wicking of moisture cannot occur.

3.6.3.1 Results of Point-Load Repository with Backfill

The point-load repository design is compared for no-backfill (the reference-repository design), crushed tuff backfill, and quartz-sand backfill using the base-case hydrologic property set (DTN LB971212001254.001). Averaged temperature and relative-humidity results are presented for each of the repository subregions for each of the designs considered. The results of this design

option study are obtained using the TH multiscale modeling and abstraction method for the LTA climate state.

Figures 3-133 through 3-138 indicate the average temperature and relative humidity for each repository subregion before and after backfill. Although the temperature differences predicted at the surface of the waste package after backfill are small for different fill materials, the difference in temperature for backfill and no-backfill cases is quite large. The average temperature increase at the time of backfill for each material is between about 70°C and 100°C. The after backfilled temperature for the crushed tuff is slightly higher than the quartz sand. The average temperature in Region SW for the quartz-sand backfill remains below 200°C. All other repository subregions produce maximum temperatures after backfill of about 210 to 220°C for a quartz-sand backfill. Crushed-tuff backfill temperatures are all somewhat above 200°C. The maximum temperatures, after a crushed-tuff backfill emplacement, are between 210°C and 240°C. As expected, the maximum average waste package temperature after backfill occurs in subregion CC. Recall that the temperature gradient through the backfill material is quite substantial (as a result of its low thermal conductivity) so that the drift-wall temperatures are all below 200°C. The increases in individual waste-package temperature at the time of emplacement may be high for some of the hotter waste packages (for example, a design-basis fuel). The results given are for the average of all waste packages contained within a given repository subregion.

Relative-humidity reduction is substantial for emplacement times after backfill emplacement. Just after backfill emplacement, the relative humidity surrounding the waste package in the crushed tuff is lower than in the quartz sand. This is not totally unexpected since the peak temperatures in the crushed tuff are somewhat higher just after backfilling occurs and the quartz sand is initially emplaced at a higher moisture content. However, it is interesting to note that at about 1,000 to 2,000 years after waste emplacement (about 900 to 1,900 years after backfill), the relative humidity of the crushed tuff emplacement drift is greater than the relative humidity of the quartz sand backfilled drift. This is a function of the rewetting properties of the fill materials. The rewetting characteristics of the crushed tuff (in particular the intragranular water potential) drive the relative humidities above those of the quartz sand, which does not have as strong a rewetting potential. The crushed tuff re-wets before the quartz sand as the waste packages cool. Note that in most cases the average repository subregion relative humidity is maintained below 85% for approximately 3,000 years or more. For the quartz sand cases, the relative humidity remains below 85% for 10,000 to 20,000 years. When compared to the reference repository design of no-backfill, this is a significant improvement while providing for much drier waste package surroundings.

Another advantage of backfill emplacement is the mitigation of rockfall processes that may alter the TH environment within the drift in an unknown way. The time and fill pattern of a rockfall rubble event will be highly uncertain (refer to sensitivity study Section 3.6.6). With the selection of an engineered backfill, one can control the bulk porosity and fill patterns adjacent to the heat-generating sources. If backfill is emplaced it reduces some of the potential uncertainties associated with rockfall events that will occur for the specified reference-repository design of open emplacement drifts.

3.6.4 Thermal-Loading Studies

Thermal loading studies for the TSPA-VA include different waste-package arrangements inside the idealized emplacement drift segment. In some cases this includes taking the base-case waste-package sequencing (as described in Section 3.5.3) and placing the canisters in an end-to-end arrangement. For this sensitivity study, only the waste package and drift spacing are altered. The waste-package types and heat outputs remain as described in Section 3.5.3. The end-to-end rearrangement of waste packages is commonly referred to as the line-loading repository design. In this case, the waste packages are separated by 0.1-meter spacing and the emplacement drift spacing is increased to approximately 56 meters. This change results in an equivalent AML, 85 MTU/acre, but a much higher lineal power load (in kW/m) and lineal mass load (in MTU/m). This design study is incorporated to assess the merits of water draining through the widely spaced emplacement drifts and away from the packages. The line-loading sensitivity analyses are performed with the TH multiscale modeling and abstraction method used to generate the base-case results.

A different thermal-loading sensitivity study takes the base-case point-load design for an 85 MTU/acre repository and places different waste packages with different heat outputs into an idealized drift segment.

For this sensitivity study, two different drifts are considered, one drift with a much hotter sequence of waste packages, the other with a much colder sequence. The waste package spacing changes as a function of MTU inside a particular waste package. The 85 MTU/acre mass load is still maintained. The hot drift segment contains some of the hottest waste packages expected to be placed in the repository. It is not thermally balanced with respect to the average repository-wide thermal load. It is much hotter. It is meant to represent a locally hot region that may result if this warmer sequence of waste packages were placed in the repository. Similarly, the cold drift segment contains some of the coldest waste packages expected to be placed in the repository. It also is not balanced with respect to the repository-wide thermal load. This sequence is meant as an approximation of a locally cold location that may occur if a sequence of low-energy-output waste packages were to be placed in the repository near each other. The waste package sequence sensitivity studies described above are implemented in three-dimensional TH drift-scale models developed to test the TH multiscale modeling and abstraction method. This analysis used a G-ECM conceptual model instead of the DKM conceptual model implemented in the TH multiscale modeling and abstraction method. All of the sensitivity studies described above are performed so that an assessment can be made of the response of the EBS to different waste-package loading strategies and different waste-package sequencing.

A final sensitivity study considers delayed thermal loading, or aging of the waste stream 10, 20, 50, and 100 years after initial waste emplacement. This study is performed at the scale of the mountain. It considers initial thermal loads much lower than the base-case simultaneous emplacement of 93-99 kW/acre.

3.6.4.1 Line-Loading Analyses

TSPA-VA focuses on the reference point-load repository design. However, preliminary analyses of design alternatives are conducted. One important option affecting the TH behavior of a

repository system is a line-load design. In this design, packages are placed as close together within drifts as practical, with drift spacing adjusted to keep the mass-loading density constant at 85 MTU/acre.

In the point-load design, waste package spacing within drifts is about the same as the half spacing between drifts. The current reference point-load design has a drift spacing of 28 meters, at a lineal mass loading of 0.588 MTU/meter. In the line-load design, waste packages are placed as nearly end-to-end as practical. The line-load design analyzed has a drift spacing of 56.6 meters and a lineal mass loading of 1.189 MTU/meter.

Point-load and line-load designs differ with respect to (1) line-average thermal loading; (2) variability of thermal loading along the drifts; and (3) drift spacing, which can be greater for the line-load design and which greatly improves the effectiveness of condensate drainage between drifts.

For the TH multiscale modeling and abstraction method used to evaluate repository design alternatives, the base-case property set, mean α_f with DTN LB971212001254.001, is used for the LTA infiltration rates. A comparison of the effects of line-load and point-load designs, and drift backfill, is made by computing the TSPA-VA performance measures over the entire repository footprint area and by computing drift-scale behavior at representative locations. Three repository-design alternatives are compared:

- Line-load and point-load with no backfill, in which the waste packages are spaced 0.1 meters apart axially (end-to-end) and the spacing between drifts is doubled to 56 meters

- Line-load and point-load with crushed-tuff backfill, in which backfill is placed between and around waste packages and does not completely fill drift

- Line-load and point-load with quartz-sand backfill, which assumes that measures are taken to prevent backfill from filling the 0.1-meters gaps between waste packages. As in the point-load backfill case, the backfill does not completely fill the drift

3.6.4.1.1 Results of Line-Load and Point-Load With and Without Backfill

The repository design option sensitivity study included investigation of two repository designs (point-load and line-load) for open, crushed-tuff-filled, and quartz-sand-filled emplacement drifts. Backfill emplacement occurs 100 years after waste emplacement. Average waste package temperature and relative humidity are compared for repository subregions SW, CC, and NE for the LTA climate. The results of this repository design study are obtained using the TH multiscale modeling and abstraction method for the higher infiltration rate LTA climate state.

Figures 3-139 through 3-141 compare the point-load (reference-repository design) to the line-load for an open emplacement drift during the LTA climate state. As specified above, the open emplacement drift is the reference-repository design. The repository subregions chosen include one with the greatest edge proximity, center, and a location that responds in-between center and edge. From the figures it is noted that the early time behavior of the line-load design indicates

very high temperatures and low relative humidities for each of the repository subregions considered. The results of the figures are for the average characteristics for a given repository subregion (i.e., region NE). For specific (hotter) waste packages (i.e., the design basis fuels in the line-load), the maximum waste package surface temperature approaches 300°C for an open emplacement drift (refer to Figure 3-149). For a backfilled drift (quartz sand), the waste package surface temperature for the design basis waste package in the line-load reached nearly 350°C (refer to Figure 3-150). The peak temperatures for the line-load design are on average 100°C or higher than the peak temperatures of the point-load design. The difference in temperature, although much reduced after peak values, persists for about the first 1,000 years after waste emplacement. After 1,000 years some relative humidity reduction exists for the line-load design; however, it is a very small difference. Relative humidities at the waste-package surface have returned to 85% at or before 1,000 years after waste emplacement.

Figures 3-142 through 3-144 compare the point-load to the line-load for an emplacement drift partially filled with a quartz-sand backfill. The change in temperature at backfill (abrupt change at 100 years) is greater for the point-load than for the line-load. This results from the fill material being isolated from the gap-spacing between line-loaded waste packages. The after-backfill average waste-package temperature is higher for the line-load cases (at each of the three repository subregions considered) since the temperature at the time of backfill is greater in the case of the line-load. The maximum average waste-package temperature after backfill for the point-load ranges from 200°C to about 220°C. The maximum average waste-package temperature after backfill for the line-load ranges from 210°C to about 250°C. Relative-humidity reduction is substantial for both cases after backfill occurs. For the line-load, average waste-package relative humidities for each of the repository subregions remains below 85% for approximately 10,000 to 20,000 years after waste emplacement. This occurs even while waste-package temperatures have dropped far below the nominal boiling point of water at the repository elevation. This is a characteristic of the low rate of rewetting potential exhibited by the quartz-sand backfill. The point-load design indicates nearly as extensive relative-humidity reduction. For the quartz-sand backfill at 100 years, the line-load design outperforms the point-load design only slightly on the basis of relative-humidity reduction alone.

Figures 3-145 through 3-147 compare the point-load to the line-load for an emplacement drift partially filled with a crushed-tuff backfill. As in the case of the quartz-sand, the change in temperature at backfill is greater for the point-load design. However, the peak temperature after backfill is much higher for the line-load case as its temperature before backfill is much higher. The maximum average waste-package temperature ranges are similar to the quartz-sand case, between 200°C and 250°C after backfill. The major difference between this case and the previous one is in the extent and duration of the relative-humidity reduction at the surface of the waste package. The crushed-tuff intragranular properties drive enhanced rewetting rates compared to the quartz-sand properties. For the crushed-tuff backfill, the relative humidity returns to 85% after about 2,000 to 3,000 years. This backfill material results in a much wetter environment near the waste packages for the cases that consider backfill. It is also interesting to note that the point-load and the line-load designs behave in a very similar manner at long times after backfill emplacement. Details associated with water content and drift relative humidity are given in the following.

Differences between the line-load and point-load designs, with respect to saturation of the rock matrix and relative humidity reduction in the NFE, are evident from Figure 3-148. The line-load causes a much greater decrease of the waste package relative humidity. For the line-load design with medium-output 21PWR waste packages, the waste package relative humidity is projected to be less than 60% at 1,000 years for a large fraction of the repository area, compared to 80% for the point-load design (Figure 3-148a and b). At 2,000 years, the area of the repository with waste package relative humidity less than 80% is much greater for the line-load than for the point-load (Figure 3-148d and e).

For further analysis of differences in drift-scale TH effects, the l5c2 location was selected for the reasons previously discussed. Three waste package types are considered, including the high-output, medium-output, and low-output types described in earlier text. The influence of repository design alternatives on relative humidity in the NFE is evident from Figure 3-149. The line-load design produces more intense heating near the drifts and more efficient condensate drainage between the drifts. The result is greater decrease of relative humidity and more persistent relative humidity reduction on the drift wall and on waste packages. The duration of decreased relative humidity is three times longer for the line-load design than it is for the point-load design. The most substantial improvement in relative humidity conditions is for the low-output HLW waste packages (Figure 3-149f) because radiative heat transfer between waste packages helps to eliminate the cold-trap effect.

There is a profound contrast in relative humidity reduction in the NFE between the line-load design with and without backfill. For medium-output waste packages in a backfilled line-load repository, the waste package relative humidity is projected to be less than 35% at 1,000 years over the entire repository (Figure 3-148c). At 2,000 years, the waste package relative humidity is less than 55% for the same design (Figure 3-148f); at 10,000 years, the waste package relative humidity is less than 75%, over the entire repository area, for the same design (Figure 3-150d). With backfill, relative humidity reduction occurs mainly within the drift backfill and not within the host rock. Consequently, the projected performance of backfill is insensitive to edge-cooling effects.

The use of backfill in the point-load design causes the waste packages to be thermally isolated. Consequently, for medium-output and high-output waste packages, drift-wall temperature increases abruptly at 100 years when the backfill is emplaced, (Figure 3-150a and Figure 3-150c). Before backfill is emplaced, thermal radiation smoothes out the heat flux and temperature along the drift wall. After backfilling, heat flux from a waste package is conducted locally, sharply increasing the temperature. The temperature increase with backfill in the point-load design is enormous for the hottest waste packages, even compared with the line-load design. By contrast, low-output waste packages produce a decrease in temperature at the drift wall after backfilling because radiative heat transfer from neighboring waste packages is eliminated (Figure 3-150e).

Radiative heat transfer between waste packages in the backfilled line-load design enables "sharing" of the thermal load, which equalizes the distribution of temperature. The result is that the low-output waste packages are much hotter and drier in line-load designs (with or without backfill) than they are in the point-load design (Figure 3-150f).

As discussed earlier, the environmental conditions on waste packages are binned according to the time required by waste packages to return to a relative humidity (relative humidity) of 85%. A relative humidity of 85% was selected because it is a typical of the critical relative humidity for atmospheric corrosion (RH_{crit}) (i.e., the value of relative humidity where atmospheric corrosion is initiated). A useful way to display the distribution of environmental conditions on all waste packages throughout the repository is to use a CCDF of the time required for waste packages to rewet to an relative humidity of 85% (Figures 3-151 through 3-152). The CCDF of waste package rewetting time is affected by three key factors:

- Edge-cooling effects—with waste packages closest to the repository edges cooling earlier, this causes them to rewet earlier than waste packages closer to the repository center. There is a gradual progression from edge-like rewetting times to center-like rewetting times.

- Repository-scale variability of percolation flux—with waste packages in areas of high percolation flux rewetting earlier than waste packages in areas of lower percolation flux. (Recall that because of the assumption that spatial attenuation of infiltration flux is negligible, the percolation-flux distribution and infiltration-flux distribution are equivalent.) The wide range of infiltration (and percolation) flux in the repository area results in a wide range of waste package rewetting times.

- Waste package-to-waste package variability of heat output—with cooler waste packages rewetting earlier than hotter waste packages. Because of the wide range of waste package heat output, there is a wide range of waste package rewetting times. For cases with engineered backfill, this factor dominates the CCDF of waste package rewetting times, particularly for the quartz-sand-backfilled, point-load design.

The CCDF of waste package rewetting time is also affected (to a somewhat lesser extent) by a fourth factor:

- Matrix imbibition diffusivity $D_{imb,m}$ of the local host rock—which is a measure of the magnitude of capillary-driven rewetting in the rock matrix, with waste packages in regions of high $D_{imb,m}$ rewetting earlier than waste packages in regions of lower $D_{imb,m}$.. Because the tsw36 (Tptpln) host-rock unit has a much higher $D_{imb,m}$ than the tsw34 and tsw35 (Tptpmn and Tptpll) host-rock units, waste packages lying in the tsw36 tend to rewet earlier.

For cases with an engineered backfill that does not strongly wick moisture back to the waste package (e.g., a well-sorted, medium-to-coarse sand), the first, second, and fourth points above are much less important than the third point. For cases without backfill and for cases with an engineered backfill that does strongly wick moisture back to the waste packages, all four factors significantly affect the CCDF of waste package rewetting time.

The TSPA-VA base-case family of hydrological property sets includes five property sets: (1) $\alpha_{f,mean}$, I, (2) $\alpha_{f,min}$, I ÷ 3, (3) $\alpha_{f,max}$, I ÷ 3, (4) $\alpha_{f,min}$, I x 3, and (5) $\alpha_{f,max}$, I x 3, where I stands for the nominal infiltration-flux map and α_f stands for the van Genuchten "alpha" parameter for

fractures. These property sets are applied to five cases that assume the present-day-climate (I) infiltration-flux map and to five cases that assume the LTA infiltration-flux map. Figure 3-151 plots the CCDF of waste package rewetting time for the $\alpha_{f,mean}$, I case for both the point-load and line-load designs with no backfill.

The influence of repository (point-load versus line-load) design on waste package rewetting time is very significant (Figure 3-151). For the present-day climate, the rewetting time for the median waste package in the line-load design is 80% greater than it is for the point-load design (Figure 3-151a), while for LTA climate, the rewetting time for the median waste package is twice that for the point-load design (Figure 3-151b). The influence of the line-load design, relative to the point-load design, is similar to a threefold decrease in the percolation flux. The greater local heat flux from the line-load drifts, and more effective condensate shedding between drifts, enable much more persistent rock dryout around the drifts, resulting in lower relative humidity on waste packages.

The influence of repository (backfill versus no backfill) design on waste package rewetting time is profound (Figure 3-152). The difference is due to thermal isolation (of a waste package) resulting from backfill of the point-loaded emplacement drift and the extensive localized heating associated with this isolation. The addition of a crushed-tuff backfill in the point-load design increases the rewetting time of the median waste package by a factor of 2.6, relative to the case with no backfill, for the present-day climate (Figure 3-152a) and by a factor of 3.7 for the LTA climate (Figure 3-152b). The addition of a quartz-sand backfill in the point-load design has a much greater effect on extending the waste package rewetting times than the crushed-tuff backfill. The addition of a quartz-sand backfill in the point-load design increases the rewetting time of the median waste package by a factor of ten, compared to the case with no backfill for the present-day climate (Figure 3-152a), and by a factor of twenty for the LTA climate (Figure 3-152b). Because of the much stronger intragrain capillary-driven wicking of moisture in the crushed-tuff backfill, relative humidity reduction is much less persistent than it is in the quartz-sand backfill case.

For medium to hot CSNF waste packages, the addition of quartz-sand backfill in the point-load design results in a substantial increase in waste package rewetting times; however, for relatively cool CSNF waste packages and HLW waste packages, the increase in waste package rewetting time is much less. The benefit of engineered backfill arises from the local temperature difference $\Delta T_{wp,local}$ between a waste package and adjacent drift wall; $\Delta T_{wp,local}$ is dependent on the local heat flux from that waste package. Because the backfilled point-load design thermally isolates waste packages from each other, hotter waste packages cannot share heat with neighboring cooler waste packages. The line-load design, which places waste packages nearly end to end, allows for efficient sharing of heat between waste packages. Consequently, the coolest waste package in the line-load design has a much greater local heater flux with which to generate $\Delta T_{wp,local}$ than even moderate heat-output waste packages in the point-load design. Consequently, the coolest (and wettest) waste package in the quartz-sand-backfilled, line-load design takes nearly 8,000 years to rewet to an relative humidity of 85% for both the present-day climate and LTA climate. Therefore, the coolest and wettest waste package in the quartz-sand-backfilled line-load design has a greater rewetting time than: (1) 37% of the waste packages in the quartz-sand-backfilled point-load design, (2) 87% of the waste packages in the crushed-tuff-backfilled

point-load design, and (3) all of the waste packages in the point-load design with no backfill. For the present-day climate, the rewetting time for the medium waste package is 15,200 years for the quartz-sand-backfilled, line-load design; 10,400 years for the quartz-sand-backfilled, point-load design; 2,700 years for the crushed-tuff-backfilled, point-load design; and 1,040 years in the point-load design with no backfill. Only the very hottest waste packages have a longer rewetting time in the quartz-sand-backfilled, point-load design than in the quartz-sand-backfilled, line-load design.

3.6.4.2 Hot- and Cold-Emplacement Drift Segments

3.6.4.2.1 Hot Segment

The hot-emplacement drift segment contains the same overall breakdown of waste-package types previously indicated in Table 3-23. The percentage breakdown of waste-package types is constrained by the controlled design assumptions document (CDA). The results of that table are repeated here for convenience. The hot drift segment includes one-half 12 PWR, three 21 PWRs, two 44 BWRs, and one-and-one-half additional waste packages. The model is a three-dimensional drift-scale model including hydrology and it is for a central repository location. In the hot-drift segment, the additional waste are co-disposal waste packages only. The coldest waste-package in this drift has an initial heat output of 4.06 kW. The heat output and waste-package spacing for the hot drift segment are given in Table 3-34. As indicated, this idealized emplacement drift segment is characterized by an AML of 85 MTU/acre and is a point-load design. The drift spacing is 28-meters. This segment assumes that the hot-waste packages are placed as they are received. It is a scenario in which a number of hot-waste packages, possibly received at the same time, are placed into the emplacement drift together.

As in the base-case drift segment, the additional wastes are placed between commercial waste packages. They do not take up their own space in the repository. The hot segment does not contain the colder direct-disposal waste package. It contains one-and-one-half co-disposal waste packages. The full co-disposal waste package is placed between the design-basis waste package and an average 21 PWR waste package. A minimum 1-meter separation distance between the ends of waste packages is maintained for the hot drift segment. The one-half co-disposal waste package is placed at the end of the drift segment adjacent to a 44 BWR waste package.

3.6.4.2.2 Cold Segment

The cold emplacement drift segment contains the same overall breakdown of waste-package types previously indicated in Table 3-23. The percentage breakdown of waste-package types is constrained by the CDA document. The results of that table are repeated here for convenience. The cold drift segment includes one-half 12 PWR, three 21 PWRs, two 44 BWRs, and one-and-one-half additional waste packages. The model is a three-dimensional drift-scale model including hydrology and it is for a central repository location. In the cold drift segment, the additional wastes are direct-disposal waste packages only. The waste package with the lowest power output in this idealized drift has an initial heat output of 0.8 kW while the hottest is the 12 PWR, which has an initial heat output of 10.5 kW. It is noted that the cold drift segment does not contain a design basis waste package in its sequence. The heat output and waste package spacing for the cold drift segment are given in Table 3-35. As indicated, this idealized

emplacement drift segment is characterized by an areal mass load of 85 MTU/acre for a point-load design. The drift spacing remains at 28-meters. This segment assumes that the cold waste packages are placed as they are received. It is an idealized scenario in which a number of cold waste packages, possibly received at the same time, are placed into the emplacement drift together.

As in the base-case drift segment, the additional wastes are placed between commercial waste packages. They do not take up their own space in the repository. The cold segment does contain the colder direct-disposal waste package; however, it does not contain the co-disposal waste package. The direct-disposal waste packages are placed between the 44 BWR waste packages. A minimum 1-meter separation distance between the ends of waste packages is maintained for the cold drift segment.

A thermal loading comparison can be made of each of the drifts, hot and cold, to the base-case drift segment described in Section 3.5.3. Table 3-36 indicates thermal loading data for each of the idealized drift segments. The power output per unit length of drift is given for each of the three (idealized) emplacement drift scenarios.

3.6.4.2.3 Comparison of Drift Segments

A comparison between drift segments given in Table 3-34 and Table 3-35 is performed using the base-case hydrologic and thermal property sets developed in DTN: LB971212001254.001 and DTN: SNT05071897001.002, respectively. Refer to Table 3-3 for the quality status of each property set. The infiltration rate applied to this sensitivity analysis is 11.5 mm/yr. It applies to a repository center location for the present-day climate.

This sensitivity study is performed with the PA (testing) drift-scale models; it is not a result of the TH multiscale modeling and abstraction method. Recall that the testing model is a three-dimensional drift-scale model including hydrology directly in its formulation. As stated in Section 3.4.1, the conceptual heat and fluid flow model in the testing approach is a G-ECM. It allows for a limited degree of fracture flow. Conversely, the TH multiscale modeling and abstraction method uses a dual permeability formulation in the LDTH model. It allows for fracture flow to occur by eliminating the capillary pressure restrictions between fracture and matrix rock. These differences in model conceptualization may result in temperature profiles, produced for this drift sequencing study, that look different than those produced for the base-case simulations given in Section 3.5.5. This is a direct result of how each model formulation handles fluid flow in the fractures and the generation and subsequent movement of steam from matrix rock to fractures. It is a function of fracture spacing and X_{fm} (fracture matrix rock interaction parameter) incorporated in a DKM but not included in the G-ECM of the testing model approach. This sensitivity analysis is meant only to provide an estimate as to the potential range of waste package variability that may result from obscure waste-package emplacement schemes. The results of this study are not carried to expected dose rates.

The base-case drift segment is compared to a hot and cold drift segment. In each case, the hottest waste package in the drift segment is compared to an average (or medium) waste package as well as to the coldest waste package in the idealized drift. Figure 3-153 indicates temperature and relative humidity for the base-case segment. For this drift segment (base case), the design-

basis fuel is hottest, the separate (direct-) disposal is coldest. The ΔT between the design-basis waste package and the direct-disposal waste package is approximately 80°C at peak values. Peak temperatures occur between about 15 and 25 years after emplacement. The boiling period lasts between 1,000-5,000 years, with the early time representative of a DKM, the later time representative of a G-ECM. After 10,000 years little waste-package variability remains. After about 1,000 years, most of the waste-package relative humidities are greater than 90%.

The "hot" drift segment compares a design-basis waste package, an average waste package, and a co-disposal waste package. In this idealized segment, the co-disposal waste package is the coldest in the group. The design-basis waste package represents the highest heat output. Figure 3-154 indicates temperature and relative humidity for the "hot" drift segment. The maximum ΔT between the design-basis waste package and the co-disposal waste package is approximately 50°C at peak values. All peaks occur at about 15 years after waste emplacement. The maximum temperature in the "hot" drift segment is about 15°C higher than the base case. The lowest temperature in the "hot" drift segment is about 50°C higher than the base case. Relative-humidity reduction is somewhat increased for the warmer drift segment; however, most of the waste packages are above 90% after 1,000 years. The boiling period is extended in this case. However, the extent of the boiling process is exaggerated by the G-ECM conceptualization.

The "cold" drift segment compares a 12 PWR, an average 21 PWR, and a direct-disposal waste package. The 12 PWR is the warmest waste package in the segment; the direct-disposal waste package emits the lowest power output. Figure 3-155 indicates temperature and relative humidity for the "cold" drift segment. The maximum ΔT between the 12 PWR waste package and the direct-disposal waste package is approximately 15°C at peak values. The maximum ΔT between the 12 PWR waste package and the coldest waste package in this segment is about 30°C. Due to the proximity of the direct-disposal waste package with respect to the 44 BWR waste package, its surface temperature is higher than both of the cold 21PWRs in this drift segment. Peak temperatures are delayed in the cold segment by about 10 to 15 years as compared to the base case-segment. The maximum temperature in the "cold" drift segment is about 70°C lower than the base case. The lowest temperature in the "cold" drift segment is about 15°C lower than the base case. Humidity reduction is substantial but less in the cold drift segment as compared to the base-case segment. After 1,000 years all waste packages in this segment have a relative humidity greater than 98%.

Figures 3-156 through 3-158 compare the design basis, average 21PWR, and the direct-disposal waste packages for common components in each of the idealized segments. The average 21 PWR is represented in each of the drift segments considered in this sensitivity study. Table 3-36 indicates that the total lineal power load is ± 0.2 kW/m from the base case in this drift sequencing study. From the figures it is clear that early time differences occur in both maximum peak temperature and the time after waste emplacement in which the peak value occurs. At late times (approximately 10,000 years), the differences in temperature and relative humidity do not persist. This would result in almost identical predictions by the waste-package corrosion models for each of the drift segments, base case, "hot," and "cold." Boiling periods are slightly extended (by 1,000 years) or reduced depending on the lineal power load. This would have the greatest

effect on the waste-package corrosion models. After 20,000 years each of the segments reproduces nearly identical waste package thermodynamic response curves.

For completeness, it is recommended in future analyses, in particular for the license application, that the drift segment study be performed using the TH multiscale modeling and abstraction method, which implements a DKM conceptual flow model. A comparison study can be used to determine the duration and extent of the formation of boiling regions predicted by a G-ECM and DKM simulations. It is fair to note, however, that even though the DKM most likely would predict a somewhat shorter duration boiling period, the trends will be entirely analogous. That is, the hot drift segment would produce a slightly longer boiling period, the cold drift a slightly shorter boiling period when compared to the base-case drift segment. The DKM producing extended cooling (which is defined as when the temperatures drop below the nominal boiling point) commence between 1,000 and 2,000 years after waste emplacement rather than about 5,000 years as predicted by the G-ECM models.

3.6.4.3 Delayed Thermal Loading

The TH calculations were all performed assuming that the waste is emplaced as it is received. A delay in emplacement or ventilating the drifts for some period of time after emplacement can affect the TH performance of the repository. If the waste is emplaced as it is received, then the initial total heat load over the entire repository would be 73.7 MW. After 20 years, this heat load has been reduced to 48.6 MW or 66% of the initial heat load and by 100 years, the total heat load has dropped to 18.8 MW or 26% of the initial heat load. During the first 100,000 years of the repository, a total of 1.5×10^{18} J of energy will be released by the waste. Of this energy, 2.5% is released in the first 20 years and 7.5% is released in the first 100 years. Clearly, even though only a few percent of the waste energy are released in the first few decades, the rate at which heat is released is so high that the early time behavior of the repository could be dramatically altered by eliminating or reducing the waste heat generated in the first 100 years.

A series of four two-dimensional mountain-scale TH simulations were performed to determine the effect of waiting for the waste to cool down before emplacing it into the repository. The simulations used the base case α_f-mean property set at the nominal I infiltration rate. (The property set DTN is LB971212001254.001 and the infiltration rates DTN is DTN GS960908312211.003; these data are qualified). The heat-generation curves were set equal to the nominal heat-generation curve except that the heat load was set equal to zero for either the first 10, 20, 50, or 100 years (the thermal loading rates DTN is SNT05071897001.004; this datum is not qualified). The air mass fraction (Figure 3-159 and Figure 3-160) and the gas-flow rates (Figure 3-161 and Figure 3-162) are plotted for all four cases and were compared to the nominal heat-loading case.

The air mass fraction at the center of the repository increased as the emplacement delay time increased. With no delay in waste emplacement, the air mass fraction dropped below 10^{-7} for almost 700 years. With a 50-year delay in emplacement, the minimum air mass fraction was 0.008 and with a 100-year delay in waste emplacement, the minimum air mass fraction rose to 0.015. At the edge of the repository, the same trend of increased air mass fractions with increased emplacement delay times was seen. With no delay, the minimum air mass fraction was 0.001 at 33 years. With a 50- and 100-year delay in emplacement, the minimum air mass

fractions were 0.48 and 0.61 respectively. Clearly, it is the rate at which the heat from the waste is released rather than the total quantity of energy released that drives the reduction in air mass fraction in the repository.

At the "center" of the repository and with no delay in the emplacement of the heat-generating waste, the gas flux peaked at ~4×10^{-6} kg/m^{2}s twenty years after waste emplacement. The gas flux then decreased to reach ambient conditions after 100,000 years. For a ten-year delay in waste emplacement, the gas-flux curve rises sharply for twenty years until it reaches the gas-flux curve for the case with no emplacement delay. The gas-phase flux curves are almost indistinguishable from each other after 30 years. Other delayed heat-loading cases also showed similar behavior; rising quickly until the gas flux reaches the gas-flux curve for the case with no emplacement delay and then following that curve until the system reaches ambient conditions. At the edge of the repository before 2,000 years, the gas fluxes were always higher for cases with smaller waste emplacement delay times. After 2,000 years, the gas fluxes were nearly identical.

These results show that a delay in heating time will result in a higher air mass fractions and identical or smaller gas fluxes at center and edge locations in the repository. Future studies in thermal loading strategies should include emplacement with ventilation (limited amount of heat released into the repository) for varying periods of time as well as delayed thermal loading combined with uneven loading of the waste (higher loading at the edge of the repository).

3.6.5 Non-Isothermal Seepage Into Drifts

The base-case seepage abstraction used for TSPA-VA is described in Sections 2.4 and 2.5 in Chapter 2 of the TSPA-VA Technical Basis Document. A detailed description of the assumptions applied to the drift seepage study performed for TSPA-VA is found in Chapter 2. One of the assumptions used in developing it was that effects of temperature could be neglected. In this subsection, we present results of a simple abstraction for including TH effects in the seepage calculation. A method such as this could be used in future TSPAs if it were found necessary to include nonisothermal seepage effects. Two important caveats are: (1) This method should be tested against more rigorous process modeling. (2) Only transient TH effects are included; drift collapse because of thermal stresses and permanent alteration of hydrologic properties by mechanical or chemical coupled processes are not considered.

The abstraction for this sensitivity analysis is based on the following method. The seepage abstraction defines the amount of seepage as a function of the fracture component of percolation flux (the matrix flow will not seep into drift openings because of high capillary suction). The abstraction was developed from steady-state, isothermal drift-scale flow calculations, but a plausible way to approximate it for a non-steady, nonisothermal situation is to take the local fracture flux above a drift in a TH calculation and use that flux in the seepage abstraction model to calculate the amount of seepage. A second factor that is applied is the drift-wall temperature. In detailed drift-scale TH calculations that have been done, it was observed that no seepage occurred when the drift-wall temperature was above boiling (Nitao 1997). We assume for this sensitivity analysis that this effect is generally true, so no seepage is allowed when the drift is above boiling.

Before continuing, a little background on the seepage abstraction model is needed. The TSPA-VA seepage abstraction is inherently probabilistic because of the great uncertainty about how much seepage there will be into emplacement drifts and how it will be distributed spatially. In the seepage abstraction, two quantities are calculated as functions of the fracture percolation flux. The two quantities are *seepage fraction*, which is the fraction of waste packages contacted by water seeping into drifts, and *seep flow rate*, which is the rate of flow of water dripping onto one of the waste packages that has seepage. For purposes of total-system simulation, at each value of percolation flux a probability distribution is defined for seepage fraction and for seep flow rate, and the values used for a given probabilistic realization are randomly sampled from those probability distributions. This process is described in more detail in Section 2.5.2.4 in Chapter 2 of the TSPA-VA Technical Basis Document. For the nonisothermal sensitivity analysis described here, we will just use the mean values from the probability distributions. The mean values give seepage fraction f_s and seep flow rate Q_s as simple functions of percolation flux rather than as probability distributions that vary with flux. The mean f_s and Q_s as functions of percolation flux are shown in Figures 2-109 through 2-112 in Chapter 2 of the TSPA-VA Technical Basis Document. At low values of flux, two relations for seepage vs. flux are shown in Figures 2-109 and 2-110 in Chapter 2 of the TSPA-VA Technical Basis Document, the "initial" curves that are obtained directly from results of process modeling and the "final" curves that have been adjusted to take into account spatial variability of percolation flux when spatial-average fluxes are being used. For the analysis here, the "initial" curves are used because we are applying the relationships to flux at a particular location, not a spatial average over a large area.

To apply the seepage abstraction to a TH calculation, we use results from the PA testing G-ECM model with mean infiltration and nominal fracture alpha, for the repository-center location. The thermal percolation flux computed above the crown of the drift is obtained from the PA testing models described in Section 3.6.1. The percolation flux from three meters above the drift is taken from the TH model and used as input to the seepage abstraction model. Note that total percolation flux was used because fracture flux was not available, but the two differ by a small amount. As mentioned above, the seepage is also reduced to zero when the drift-wall temperature is above boiling.

The seepage fraction and seep flow rate calculated in this way are shown in Figure 3-163 and Figure 3-164. The results for seepage above three waste packages from the model are shown: for flux and temperature taken from above the design-basis 21-PWR package, from above an average 21-PWR package, and from above the direct-disposal N-reactor package. The results show a pulse of enhanced seepage as a result of condensate drainage for a few thousand years. The seepage during the pulse is not increased dramatically, but the seepage fraction does increase by about a factor of two and the seep flow rate increases by about a factor of three. The results are slightly different for the three different waste packages, with the hottest one (the design-basis package) staying dry for longest and the coolest one (the N-reactor package) being the first to rewet. There is also a brief early pulse of condensate seepage right after emplacement that is not shown in the figures because it occurs before 10 years.

3.6.6 Rockfall and Thermal-Hydrologic Response

This sensitivity study includes a rubble fill surrounding the waste packages as a result of the collapse of the emplacement drift wall after emplacement of heat-generating wastes. We will not

consider damage to the waste package (if any) as a result of rockfall-rubble impact. It is assumed that drift-wall collapse occurs simultaneously and uniformly at a predetermined time after waste emplacement. We will consider this analysis only as it pertains to a change in the environment (such as temperature, relative humidity, and liquid saturation) surrounding the waste package after rockfall. Therefore, we will look at this problem only in terms of the thermal and hydrologic changes at the waste-package surface as a result of direct contact of a "non-engineered backfilling process." The process considered is an idealized event in which drift instability as a result of thermal stresses includes a complete drift wall collapse. The study does not consider the mechanical processes that may occur, only the processes that result in a new drift environment.

This sensitivity analysis is performed using the preliminary base-case hydrologic property set, DTN: LB971100001254.002, for the nominal I infiltration rate of 11.5 mm/year. This infiltration rate corresponds to a repository center location. The thermal property set is from the base case, DTN: SNT05071897001.002. The rockfall analysis uses the PA testing models developed above. It is a three-dimensional, TH, drift-scale model including the base-case waste-package sequencing established in Section 3.5.3. Recall that the conceptual flow assumption used in this model is a G-ECM.

It is assumed in this modeling study that rockfall occurs uniformly at 1,000 years after the emplacement of heat-generating wastes. It occurs instantaneously in time, filling the entire emplacement drift. It is assumed in this analysis that the initially open emplacement drift (as specified by the reference repository design) is completely filled by a rockfall event resulting in a volumetric swell factor, S_{fac}.

$$S_{fac} = \frac{V_1 - V_0}{V_0} \tag{3-26}$$

where V_1 is the final volume of rock , V_0 is the initial volume of rock. The swell factor is a measure of the volumetric increase of the rubble by formation of void space resulting from rock chunks and other-sized rock fragments. Once the emplacement drift is completely filled, it is assumed that crown migration ceases. This may somewhat underestimate the total amount of crown migration moving in the direction of the ground surface. The extent of crown migration is constrained by the assumed swell factor of the rubble fill. It is inversely proportional to the swell factor, so as S_{fac} increases, the crown migration height decreases. It is further assumed that crown migration occurs vertically upward. Crown migration is the amount, vertically upward, that the top of the drift moves. Figure 3-165 is a blow-up of a cross section of the rockfall computational grid. The grid contains the waste package, the invert, the new opening in the TSw35 caused by rockfall, and the TSw35 rock. The TSw35 rock between the invert and the opening above the rock has a higher porosity than does the TSw35 elsewhere in the simulation domain. The assumptions related to crown migration height and growth can be explored in future studies; the primary thrust of this rockfall analysis is the relative contribution of conduction and convection heat transfer from the waste package surface through the rubblized zone now filling the once open emplacement drift.

3.6.6.1 Heat Transfer Modes in Rockfall Rubble

A swell factor, S_{fac}, of 1.0 (for example, 100%) is assumed for this sensitivity study on the TH effects of rockfall. This value of S_{fac} is chosen as an upper bound on the swell factor. It is selected so as to reproduce heat-transfer rates (from the waste-package surface through the rockfall) that may potentially be at a minimum. A complete analysis of the rockfall issue may include consideration of S_{fac} in the range of 25% # S_{fac} # 65%. The swell factor is related to rockfall void porosity (of the rubblized zone completely surrounding the waste packages), ε , by:

$$\varepsilon = \frac{S_{fac}}{1 + S_{fac}} \tag{3-27}$$

It is assumed that the swell factor (and resulting ε)is uniformly distributed in the rockfall zone. Specifically, this implies that processes that redistribute fines to the bottom and larger rocks to the top (of the fill) are not taken into consideration. Using the assumed value for swell factor, the resulting rockfall void porosity is ε =0.5. This value of void porosity helps constrain the thermal conductivity of the rubblized zone as well as a range for the bulk permeability through the fill.

With the rockfall void porosity, ε and the intrinsic porosity of the rocks, ϕ_m, abulk porosity was defined in a similar manner as in an equivalent continuum approach:

$$\phi_b = (1 - \varepsilon)\phi_m + \varepsilon \tag{3-28}$$

where ϕ_m is the intrinsic matrix-rock porosity. The bulk porosity of the rubble zone is computed for a matrix porosity of ϕ_m = 0.115 as 0.5575. With this information an effective thermal conductivity of the fill is obtained.

3.6.6.1.1 Thermal Conductivity

Assuming a Hadley weighted average (Kaviany 1991, pp. 126), the effective thermal conductivity is a function of the bulk porosity (= 0.5575), the matrix solid thermal conductivity (assumed nearly dry = 1.2 W/m-K), and the thermal conductivity of the fluid in the rockfall void spaces, assumed to be air (= 0.03 W/m-K). For the range of values specified, the effective thermal conductivity of the rockfall region directly surrounding intact waste packages is approximately 0.16 W/m-K. This is similar to a geometric mean as an effective thermal conductivity, although it is slightly higher. Recall that the rockfall rubble is not an engineered backfill with a predetermined number of contact points (for example possibly determined by a material sieve, etc). It is a result of falling pieces of rock of many different sizes possibly dictated by intersecting fractures or other features.

3.6.6.1.2 Bulk Permeability

Since the effective thermal conductivity computed above is quite low, it is reasonable to assume that the convective component of heat flow (through the rubble zone) will take on an added

importance. For an open drift, radiation heat transfer is the dominant mode of heat exchange between waste package and drift wall. All other modes are essentially negligible. For a rubble-filled drift, thermal conduction is the dominant mode only at a much lower rate than radiant heat transfer. A range of bulk permeabilities has been considered in the rockfall models.

The convective component of heat transfer in the rubblized zone is proportional to the effective bulk permeability through the rockfall. The following range of bulk permeability through the rubblized zone is given in Table 3-37.

3.6.6.1.3 Other Void Space Properties

The "fracture-like" properties of the rockfall-rubble void spaces are assigned the following properties associated with capillary-pressure characteristics of the opening. The parameters are given in Table 3-38. The intrinsic matrix properties of the rockfall rubble are identical to the tsw5 model unit in DTN: LB971100001254.002.

3.6.6.2 Thermal-Hydrologic Results of Rockfall

The results of a rockfall analysis with the assumptions listed above are given in Figures 3-166 through 3-171. Temperature, relative humidity, and liquid saturations are displayed at the waste-package surface for a high-, medium-, and low-thermal-output waste-package. It is assumed that rockfall occurs 1,000 years after waste emplacement. The figures also indicate waste package response curves for the reference repository design (for example, designated as open drift without an engineered backfill).

In general, after rockfall occurs, temperatures increase while relative humidities decrease. The magnitude of change depends on the waste-package thermal output at the time of rockfall. The design-basis-fuel, waste-package surface temperature increases by approximately 60°C about 50 years after rockfall occurs. The average 21PWR waste-package surface temperature increases by about 40°C. The direct-disposal waste-package surface temperature increases by about 6°C. As indicated by the cooling curves after the rockfall event, the convective component of heat transfer does not significantly reduce the temperature at the waste-package surface. For the 100,000-darcy case, the cooling associated with this high bulk permeability only reduces the maximum temperature spike (when compared to the 7 darcy rockfall rubble case) by about 5°C for the design-basis waste package. Approximately 2,000 years after rockfall (for example, 3,000 years after waste emplacement) the differences in temperature for differing bulk permeabilities are considered negligible for the hottest waste package. For the other waste packages considered, enhanced cooling resulting from increased heat transfer by convection is negligible for all times after rockfall occurs.

The relative humidity quickly increases to 100% (just after rockfall) because the incoming rock has some (S_L approximately 0.2) water associated with it. With heating of the rubble fill, relative humidity of the design-basis waste package is driven back down to about 38% (from about 88%) for a period of about 4,000 years of reduced relative humidity. After this period, the relative humidity of the waste package is higher than if the drift remains open. For the cooler waste packages, the same trends are seen, but the time period for relative humidity reduction (after

rockfall) is much shorter. In addition, the maximum reduction in relative humidity is somewhat reduced.

Figure 3-172 indicates that liquid saturation of the rockfall rubble that is directly in contact with the waste packages. The increase in liquid saturation is a result of the moisture carried into the drift by the rockfall rubble. Some drying occurs as the waste canisters are still at elevated temperatures. The rockfall rubble saturation asymptotically approaches a liquid saturation of 0.1.

The rockfall sensitivity study was performed using the three-dimensional drift-scale TH model designated as a testing model. This model is used in the rockfall sensitivity studies instead of the TH multiscale modeling and abstraction method because time is limited limitations. This model is representative of a center repository location. The results of this study are not carried to dose-rate calculations. It is a study on TH conditions only. Future studies will incorporate different swell factors, including a range of crown migration heights for each S_{fac}. Additionally, different rockfall times should be considered for completeness. From the current study, the influence of convection heat transfer in the rubble zone did not vary all that much for the selected values of bulk permeability given in Table 3-37.

3.6.7 Sensitivity Studies Associated with Mountain-Scale Models

The two-dimensional mountain-scale TH base case and the property set sensitivity studies presented earlier in this chapter were all performed using the same simulation domain and the same boundary conditions (See Section 3.4). The sensitivity studies presented here investigate the effect of the selection of the boundary conditions used and other assumptions on the TH feeds to the Near Field Geochemical Environment. The air mass fraction and gas flux plots at center and edge locations are presented for all of the sensitivity studies and compared with those from the nominal TH simulations.

3.6.7.1 TH Results of Increased Horizontal Permeability in the Repository Elements

In the base-case simulations, the repository was modeled by placing the heat directly into the mountain without disturbing the permeability field of the host rock. Since the center and edge of the repository will heat and cool at different rates, gas-phase flow may occur up and down the drift, depending on the local pressure in the repository. A sensitivity study was run to study the effect of increasing the horizontal bulk permeabilities in the repository elements. The sensitivity study was performed using the base case α_f-mean (DTN LB971212001254.001; these data are not qualified) property set and increasing the bulk horizontal permeability in the repository host rock (tsw35 unit) three orders of magnitude (from 0.91 to 910 darcy). The infiltration rate was the nominal present-day infiltration rate (DTN GS960908312211.003; these data are qualified).

The air mass fractions at center and edge locations for the sensitivity study, with increased bulk permeability in the vertical direction in the drift elements, are presented in Figure 3-172 and Figure 3-173. The air mass fraction time-histories for the base-case α_f-mean simulations are also presented (curve is labeled "Nominal Properties") for comparison. At the center of the repository, the air mass fraction looks similar to the nominal case for the first 200 years of the simulation. The air mass fraction minimum at 400 years is not as low as it is for the nominal

case. At the edge of the repository, the air mass fraction is lower than the nominal case between 10 and 1,000 years. The difference between the air mass fraction at the center and the edge is much smaller than for the nominal case.

The gas fluxes at center and edge locations for the sensitivity study with increased drift horizontal bulk permeability are presented in Figure 3-174 and Figure 3-175. The gas flux time-histories for the base-case α_f-mean simulations are also presented (curve is labeled "Nominal Properties") for comparison. At the center of the repository, the vertical flux is dominant at early time and horizontal gas flux is dominant at late time. The horizontal flow alternates flowing east and west during the thermal perturbation. At the edge of the repository, the gas flux is almost one order of magnitude greater than the nominal case starting five years after the emplacement of the waste. Before 1,000 years, the horizontal gas flux is primarily outward away from the center of the repository; and after 1,000 years, the horizontal gas flux is inwards towards the center of the repository. Gas flow away form the center of the repository before 1000 years explains the trends that are seen in the air mass fraction plots; gas with a low air mass fraction will flow from the center of the repository to the edge of the repository resulting in a reduction the air mass fraction levels simulated at the edge of the repository.

3.6.7.2 TH Results of Increased Horizontal Permeability in the Repository Elements and Open Drifts

A sensitivity study was run to study the effect of increased bulk permeability in the vertical direction in the drift elements that are connected to the outside environment. This study is an extension of the previous sensitivity study except that it was assumed that both ends of the drift are connected to the outside environment. For this sensitivity, a constant-pressure source/sink was placed at both ends of the repository and the horizontal permeability in the repository elements was increased so that the overall pressure inside the repository would remain essentially constant throughout the duration of the simulation. The sensitivity study was performed using the base case α_f-mean (DTN LB971212001254.001; these data are not qualified) property set and increasing the bulk horizontal permeability in the tsw35 unit five orders of magnitude (from 0.91 to 91,000 darcy). Gas (steam and air) was allowed to leave at the east-most and the west-most repository element when the pressure tried to rise, and air was allowed to enter those same elements when the pressure tried to drop. The infiltration rate was the nominal present-day infiltration rate (DTN GS960908312211.003; these data are qualified).

The air mass fraction at center and edge locations for the sensitivity study with increased bulk permeability in the vertical direction in the drift elements and open drifts are presented in Figure 3-176 and Figure 3-177. The air mass fraction time-histories for the base-case α_f-mean simulations are also presented (curve is labeled "Nominal Properties") for comparison. At the center of the repository, the air mass fraction never drops below 0.07. At the edge of the repository, the air mass fraction never goes below 0.78.

The gas flux at center and edge locations for the sensitivity study with increased bulk permeability in the vertical direction in the drift elements and open drifts are presented in Figure 3-178 and Figure 3-179. The gas-flux time-histories for the base-case α_f-mean simulations are also presented (curve is labeled "Nominal Properties") for comparison. The gas

flux, which is mostly in the horizontal direction, is much higher for all time than during the nominal simulation.

Modeling the repository as being open to the environment resulted in a higher reduction in the water saturation around the repository than was seen in the base-case α_f-mean nominal I infiltration simulation. This trend is expected as the water vapor created by the waste packages could easily leave the simulation domain. Since the water vapor was allowed to exit the domain through the sinks at the ends of the repository, the constant temperature reflux zone above the repository was much smaller than in the base-case α_f-mean nominal I infiltration simulation.

3.6.7.3 TH Results of Increased Fracture Permeability

The development of the vertical fracture permeabilities is described in Chapter 2 of the TSPA-VA Technical Basis Document. In the Topopah Spring Tuff unit, where pneumatic data exist, the vertical fracture permeability is approximately ten times the horizontal fracture permeability. Because of the absence of pneumatic data in the bottom of the Topopah Spring Tuff unit, the vertical fracture permeabilities in the property sets may be lower than their actual value. A sensitivity study was performed using the preliminary base case nominal I infiltration (DTN LB971100001254.002; these data are qualified) property set but setting the vertical fracture permeabilities in the tsw35, tsw36, and tsw37 units to equal ten times the horizontal fracture permeability in those units. This sensitivity study used the nominal present-day infiltration rate.

The air mass fraction at the center and edge location of the repository for the increased fracture vertical-permeability sensitivity study are presented in Figure 3-180 and Figure 3-181. The air mass fraction time-histories for the preliminary base-case simulations are also presented (curve is labeled "Nominal Vertical K") for comparison. At the center of the repository, the air mass fractions for the two cases matched up well for all time. At the edge of the repository, the air mass fraction for the case with increased bulk permeability in the vertical direction in the drift elements was lower between 20 and 1,000 years.

The gas flux at the center and edge location of the repository for both the nominal case and the case where there is increased bulk permeability is presented in Figure 3-182 and Figure 3-183. The gas-flux time-histories for the preliminary base-case simulations are also presented (curve is labeled "Nominal Vertical K") for comparison. The gas phase flux for the two cases do not differ significantly.

3.6.7.4 TH Results of Isotropic Permeability Field in Each Unit

A sensitivity study was run to investigate the effect of having an isotropic permeability field in each geologic unit. The gas flow fields in the base-case simulations showed strong vertical gas flows and weak horizontal gas flows. There are two mechanisms that would cause this behavior. First, since heated gas and steam will rise as a result of gas-density gradients, it is expected that much of the flow will be vertical. Second, since the vertical bulk permeability is higher than the horizontal bulk permeability in the host rock region (the Topopah Spring unit), gas flow may still naturally preferentially flow vertically rather than horizontally. The sensitivity study was performed using the base case α_f-mean (DTN LB971212001254.001; these data are not qualified) property set and increasing the bulk horizontal permeability to equal the bulk vertical

permeability in all of the rock units where the permeability was not already isotropic. The infiltration rate was the nominal present-day infiltration rate (DTN GS960908312211.003; these data are qualified).

The air mass fractions at the center and edge locations of the repository for isotropic permeability field in each geologic unit sensitivity study is presented in Figure 3-184 and Figure 3-185. The air mass fraction time-histories for the base-case α_f-mean simulations are also presented (curve is labeled "Nominal Properties") for comparison. The differences between the air mass fraction time-histories of the nominal simulation and the sensitivity study are mainly between 200 and 1,000 years. At the center of the repository, the air mass fractions are higher in the sensitivity study than in the nominal case. At the edge of the repository, the air mass fractions are lower in the sensitivity study than in the nominal case.

The gas fluxes at the center and edge locations of the repository for isotropic permeability field in each geologic unit sensitivity study are presented in Figure 3-186 and Figure 3-187. The gas-flux time-histories for the base-case α_f-mean simulations are also presented (curve is labeled "Nominal Properties" for comparison. The gas flux at the center of the repository for the sensitivity study is very similar to that from the nominal case. The gas flux at the edge of the repository for the sensitivity study is very similar to that from the nominal case for the first 1,000 years and then it is higher by a half order of magnitude after 1,000 years.

3.6.7.5 TH Results of Raising the Water Table as a Result of A Climate Change

In TSPA-VA, the climate at Yucca Mountain is assumed to move between three possible climate states (see Section 2.2.1 in Chapter 2 of the TSPA-VA Technical Basis Document for more details). The TH model assumes that, in the time scale that transient TH effects are important, only the present-day and the LTA climate state will occur. The two-dimensional, mountain-scale simulations at the LTA conditions were modeled by increasing the infiltration rate to LTA values. The water table is expected to rise by 80 meters as a result of the increased infiltration rate. This increase in the water-table level was ignored in the two-dimensional, mountain-scale TH studies. A sensitivity study was performed to determine how this assumption would affect the TH feeds to the Near Field Geochemical Environment Model. The sensitivity study was performed using the preliminary base case (DTN LB971100001254.002; these data are qualified) property set and removing the bottom 80 meters from the simulation domain. The infiltration rate was the long term average infiltration rate (DTN GS960908312211.003; these data are qualified).

The air mass fractions at the center and edge locations of the repository for the high-water-table, temperature-sensitivity study for high-water-table temperature is presented in Figure 3-188 and Figure 3-189. The air mass fraction time-histories for the base-case α_f-mean simulations are also presented (curve is labeled "Nominal Mesh") for comparison. There is very little difference between the air mass fraction time-histories at the center or at the edge of the repository when the full (nominal) mesh is used or when the smaller mesh is used.

The air mass fractions at the center and edge locations of the repository for the high-water-table, temperature-sensitivity study for high-water-table temperature is presented in Figure 3-190 and Figure 3-191. The gas-flux time-histories for the base-case simulations are also presented (curve

is labeled "Nominal Mesh") for comparison. There is very little difference between the gas flux time-histories at the center or at the edge of the repository when the full mesh is used or the smaller mesh is used.

3.6.7.6 TH Results of Having a Higher Water-Table-Temperature Boundary Condition

In all of the TSPA-VA two-dimensional, mountain-scale TH simulations, the water-table temperature was set at a constant 32°C. An alternative and more computationally demanding approach would be to extend the simulation domain through the water table, allowing the water-table temperature to rise as water heated by the repository enters the SZ. A sensitivity study was performed to determine if this boundary condition used will impact the TH feeds to the Near Field Geochemical Environment model. For this study, it was assumed that if changing the water table temperature did not affect the air mass fractions or the gas flow rates, then the water-infiltration rates and thermal conduction parameters result in a weak thermal connection between the repository and the water table. If this thermal connection is weak, then it would not be necessary to expand the simulation domain to include the SZ. The sensitivity study was performed using the preliminary base case (DTN LB971100001254.002; these data are qualified) property set and the water-table element temperature increased by 10°C to 42°C. The infiltration rate was the present-day nominal I infiltration rate (DTN GS960908312211.003; these data are qualified).

The air mass fractions at the center and edge locations of the repository in the sensitivity study for the higher temperature of the water table are presented in Figure 3-192 and Figure 3-193. The air mass fraction time-histories for the preliminary simulations are also presented (curve is labeled "Nominal Water Table Temp") for comparison. The air mass fractions at both the center and the edge are slightly lower when the water table is kept at a higher temperature than in the nominal case.

The gas fluxes at the center and edge locations of the repository in the sensitivity study for the higher temperature of the water table are presented in Figure 3-194 and Figure 3-195. The gas-flux time-histories for the preliminary base-case simulations are also presented (curve is labeled "Nominal Water Table Temp") for comparison. The gas flux at both the center and the edge are the same or slightly higher when the water table is kept at a higher temperature than in the nominal case.

3.6.8 Coupled Processes

3.6.8.1 Thermal-Hydrologic-Mechanical Coupled Processes

Simulations of THM behavior of the potential repository at Yucca Mountain are presented in this section. The results of past thermal-mechanical simulations have been coupled to present TH simulations. Zones of altered rock are taken from thermal-mechanical simulations of Mack et al. (1989), to identify regions where the fracture aperture either increased or decreased by a factor of two. These altered regions are used as a reference in the present study to locally update fracture properties at five discrete times (25, 50, 100, 250, and 500 years) during the TH simulation. Comparisons are made between altered and unaltered TH simulations during approximately 700 years of heating. Results showed that the altered and unaltered simulations produce similar

trends in fracture flow, liquid saturations, and temperatures. The fracture flow at and below the repository is increased by up to several orders of magnitude in response to condensate drainage in both cases. However, in the altered case, the increased flow in the CHn persists longer than in the unaltered case.

These simulations include movement normal to the fractures. The movement includes both opening and closing. The mechanical interaction due to shear movement is not included in this analysis. It is noted that shear movement may have more lasting impacts on the fracture system than does normal movement. This may lead to enhanced horizontal fracture permeability which cannot be included in a one-dimensional TH model simulation.

3.6.8.1.1 Description of the Process of Thermal-Mechanical Influence on Hydrology

Previous investigators have simulated the TH behavior of the potential repository at Yucca Mountain, Nevada. Simulations of heat and water flow in the UZ during the thermal perturbation are required in order to understand the potential impacts of heating on radionuclide transport through the subsurface. In early studies, ECMs of heat and water flow through the fractured tuffaceous rock were used because of their computational efficiency and simple representation of fracture-matrix interaction (Tsang and Pruess 1987; Buscheck and Nitao 1993a). Recently, DKMs have been employed to explicitly model fractures and examine their role in augmenting water flux during post-waste-emplacement heating (Ho et al. 1997). However, few studies have examined the effects of mechanical changes in the fractured rock on the hydrologic response of the system. Expansion of the rock matrix caused by heating can create stress in the rock and may induce changes in the fracture apertures (Mack et al. 1989). These changes can affect the amount of flow that occurs in the fractures and, subsequently, through the entire system. These hydrologic changes can, in turn, affect the thermal behavior, which governs the mechanical changes of the rock. Although this complex behavior would require a simultaneous solution of THM equations and processes, this analysis presents a weakly coupled process that describes THM behavior of post-waste-emplacement heating conditions. Results of "one-way" THM simulations are presented, and implications for long-term performance are made based on the results of this study.

3.6.8.1.2 Modeling Approach

The effects of thermal-mechanically induced changes in fracture apertures are included in TH simulations of post-waste-emplacement behavior through a weakly coupled process. Information from thermal-mechanical simulations is passed in a "one-way" fashion to TH simulations at discrete times. Material properties in the TH simulations are updated at these prescribed times to reflect the thermal-mechanical changes to properties such as fracture permeability, moisture potential, and porosity. The results of these THM simulations are then compared to unaltered TH simulations to determine the effects of mechanical changes on hydrologic behavior. The following sections provide a detailed description of this process.

Thermal-Mechanical Model

In Mack (1989), the thermal-mechanical behavior of Yucca Mountain was simulated using the thermoelastic boundary code HEFF (Brady, 1980; Brady, 1988). Two-dimensional models of an

east-west cross-section of Yucca Mountain were used in their analysis. The rocks were assumed homogeneous and isotropic with properties corresponding to that of the Topopah Spring unit (MacDougall et al. 1987). An initial heat load of 80 kW/acre was assumed, with thermal decay characteristics specified in Peters (1983).

The intent of their work was to identify zones of "significant modification" resulting from heat emission and repository construction. They define a "significant modification" to be a change in joint aperture by a factor of two. This would result in a change in the bulk fracture permeability by nearly an order of magnitude using the cubic law. They generated two-dimensional plots of regions where the joint apertures changed by a factor of two at 25, 50, 100, 250, and 500 years of heating. The extent of these zones was measured vertically from the center of the repository at each time for use in the present one-dimensional TH analysis.

Figure 3-196 plots the zones of compression (aperture decreases by a factor of two) and zones of tension (aperture increases by a factor of two) along a one-dimensional transect at each of the five times. It should be noted that the zones of compression and tension were mapped onto the one-dimensional transect assuming that the elevation of the water table, repository, and ground surface are located at an elevation of 731 meters, 1,071 meters, and 1,292 meters. Four major stratigraphic units corresponding to this one-dimensional transect are also shown in Figure 3-196. The zone of compression, in which the fracture apertures decrease by a factor of two, are shown to increase symmetrically in size above and below the repository as time increases. The zones of tension, where the fracture apertures increase by a factor of two, are located primarily above the repository and diminish in size as time increases. More detailed explanation about the nature, extent, and location of these modified zones as a result of the thermal-mechanical simulations can be found in Mack et al. (1989).

Thermal-Hydrologic Model

A one-dimensional DKM is used to simulate the TH response of the potential repository at Yucca Mountain. The numerical code used in this study is TOUGH2 (Pruess 1991, 1987), which simulates multiphase, multidimensional, nonisothermal transport of air, heat, and water in fractured and porous media. The DKM conceptual model of flow through fractures has been shown to allow significant flow through the fractures as a result of condensate drainage from heating and transient flow (Ho 1997; Altman et al. 1996; Ho et al. 1995), and may potentially show different TH responses to changes in fracture apertures.

The one-dimensional model used in the TH simulations consists of 28 fracture elements and 28 matrix elements. It is located at an easting coordinate of 171,270 m, which corresponds to the location of borehole SD-9. The elevation of each of the 28 fracture and matrix elements is depicted in Figure 3-196 by symbols that also denote whether the corresponding fracture element has been altered due to thermal-mechanical effects. An infiltration of 3.6 mm/year (7.76×10^{-4} kg/s) is applied to the top of the domain in the fractures (an infiltration rate consistent with the NE edge of the repository outline), and steady-state ambient conditions are established before heating begins. Figure 3-197 shows a plot of the simulated steady-state ambient matrix saturations, along with the measured data for SD-9. Good agreement is achieved, confirming the calibration of the hydrologic data in the 22 defined stratigraphic units. Detailed information on the equilibration process for temperatures and pressures can be found in Ho et al. (1996). After

steady-state conditions are established, heat is applied to the repository element located at 1071 meters with an initial heat load of 80 kW/acre, commensurate with the thermal-mechanical simulations. Two TH analyses are performed using TOUGH2: (1) an unaltered simulation using the base-case properties supplied by LBNL, (Bodvarsson et al. 1997), and (2) an altered simulation using modified properties in the zones described by the thermal-mechanical simulations. The procedures for performing each analysis are described in the following section.

Thermal-Hydrologic-Mechanical Coupling

The results of the thermal-mechanical simulations plotted in Figure 3-196 are used to update fracture properties in TH TOUGH2 simulations at each of the five discrete times shown. The following expressions are used to describe changes to fracture porosity, ϕ_f, fracture permeability, k_f, and fracture air-entry pressure, α, (van Genuchten alpha) in regions where the apertures have either increased or decreased by a factor of two:

$$\phi_f = \frac{b}{D} \tag{3-29}$$

$$k_f = \frac{b^2}{12}\phi_f = \frac{b^3}{12D} \tag{3-30}$$

$$\alpha = \frac{b}{2\sigma} \tag{3-31}$$

where b is the fracture aperture (m), D is the fracture spacing (m), and σ is the surface tension of water (N/m). Equations (3-29) and (3-31) show that for changes in the fracture aperture by a factor of two, the porosity, ϕ_f, and van Genuchten alpha, α, will also change by a factor of two. However, the bulk fracture permeability, k_f, changes by a factor of eight. These parameter alterations, defined spatially and temporally by the zones shown in Figure 3-196, are incorporated in the TH analysis using six sequential TOUGH2 simulations. The initial simulation, from 0 to 12.5 years, uses unaltered hydrologic properties. The five subsequent simulations use the altered properties defined by Equations (3-29) through (3-31) at locations specified by the zones shown in Figure 3-196. The properties are updated accordingly in the five subsequent simulations at the beginning of each simulation, which span the following ranges in time: 12.5–37.5 years, 37.5–75 years, 75–175 years, 175-375 years, and 375-750 years. The results of this "altered" TH simulation are then compared to the results of a TH simulation that use the unaltered properties throughout the entire 750-year duration. It should be noted that in both simulations, convergence problems prevented the runs from reaching 750 years in 9,000 time steps. The unaltered run was able to reach nearly 600 years of simulated time, while the altered run was able to reach nearly 700 years.

3.6.8.1.3 Results

Liquid flows through the fractures at three locations is plotted in Figure 3-198 as a function of time for both the altered and unaltered simulations. The unaltered simulation shows that the flows in the fractures at the three locations (into the drift, in the TSw below the repository, and in the CHn) exhibit similar trends. Condensate drainage increases the flow in the fractures by up to

several orders of magnitude during the first 100 years, but the flow decreases towards ambient values by 1000 years. The altered simulation shows similar behavior in Figure 3-198. The only significant difference is in the CHn, where the increased fracture flow persists longer than in the unaltered simulation. A possible explanation may be that the reduced apertures near the repository in the altered simulation reduce the fracture α parameter (see Equation [3-3]), causing more liquid to be retained in the reduced fracture apertures because of higher capillary suction. The increased water in the fractures eventually drains to the CHn, elevating the flux over that of the unaltered case. The altered simulation also shows downward peaks at each of the five discrete times at which information is passed from the thermal-mechanical simulations. These numerical aberrations result from the abrupt change in material parameters used at the beginning of each of the five numerical simulations using updated properties.

The liquid saturations and temperatures are also similar between the altered and unaltered simulations, although small differences exist. Figure 3-199 shows the matrix and fracture liquid saturations for both the altered and unaltered cases at 500 years of heating. Examination of the fracture and matrix liquid saturations reveals that the fracture saturations are greater in the altered simulation in the vicinity of the repository. This correlates with the hypothesis that the reduction of fracture apertures near the repository allows more retention of water in the fractures as a result of increased capillary suction in the fractures. This, in turn, allows increased flow in the fractures in the CHn at later times (Figure 3-198). Figure 3-199 also shows that at 500 years, a dryout zone extends approximately 20 meters above and below the repository.

Figure 3-200 shows the temperature profile for both the altered and unaltered cases at 500 years of heating. Both cases show a large region of boiling, and heating is slightly greater above the repository, indicating a significant amount of heat transfer by natural convection. The altered simulation yields slightly higher temperatures at and below the repository and lower temperatures above the repository. These slight discrepancies are likely as a result of the reduced fracture apertures in the compressed zone in the vicinity of the repository. The reduced fracture apertures affect not only the saturation distributions in the fractures and matrix as discussed earlier but also the natural convection of gas. At 500 years of heating, the fracture permeability is decreased both above and below the repository by nearly an order of magnitude. Therefore, the amount of heat transferred by natural convection away from the repository is reduced. The resulting temperature profile in the altered TH simulation is more symmetric about the repository and is consistent with a reduced convection scenario.

3.6.8.1.4 Conclusions

The results of thermal-mechanical simulations have been coupled to TH simulations of the potential repository at Yucca Mountain. Past thermal-mechanical simulations (Mack et al. 1989) presented results that identified zones of altered rock where the fracture aperture either increased or decreased by a factor of two. These altered regions were used in the present study to update fracture properties at five discrete times (25, 50, 100, 250, and 500 years) during the TH simulation. The properties that were updated as a result of the changes in fracture apertures were fracture porosity, bulk fracture permeability, and fracture air-entry pressure (van Genuchten alpha parameter). Comparisons were made between altered and unaltered TH simulations during approximately 700 years of heating.

Results showed that the altered and unaltered simulations produced similar trends in fracture flow, liquid saturations, and temperatures. The fracture flow at and below the repository was increased by up to several orders of magnitude as a result of condensate drainage in both cases. However, in the altered case, the increased flow in the CHn persisted longer than in the unaltered case. It was postulated that the reduced apertures near the repository in the altered case allowed more water to be retained in the fractures because of higher capillary pressures. This subsequently produced larger fluxes through the fractures below the repository. The saturation profiles at 500 years of heating supported this hypothesis. In addition, the increased fracture flow was attenuated by 1,000 years of heating in both the altered and unaltered simulations. Finally, the temperature profiles at 500 years of heating revealed that natural convection was attenuated in the altered simulation because of reduced fracture apertures and, hence, fracture permeabilities near the repository. While the overall temperature distributions were similar between the altered and unaltered simulations, the temperatures in the altered simulation were slightly higher near the repository and more symmetric above and below the repository, indicating reduced convection in the compressed zones.

Other more direct formulations are presented in Hardin (1998, pp. 4-33 through 4-35) for permeability changes associated with shear-slip and normal deformation. For permeability changes associated with shear-slip, the resultant change is a function of a scaling exponent (relates smooth or rough fractures) and a shear offset term resulting from thermal stresses. As previously described, shear alterations tend to impact the horizontal fracture sets. For permeability changes associated with normal deformation, the resultant change is a function of the stress change perpendicular to the fractures, fracture spacing, the initial fracture aperture, and the rock-mass modulus. Each of the models presented is driven by stress changes that result from an imposed temperature field.

3.6.8.2 Thermal-Hydrologic-Chemical Coupled Processes

An analysis of THC alteration of flow pathways above and below the repository is given in Hardin (1998, pp. 5-57 through 5-67). The indicated section presents a coupled TH and geochemical reactive-transport system around a single drift. This work focused on a fracture system in the UZ containing silica. This study does not consider calcite mineralogy in the UZ fracture system. The following is a summary of the referenced analyses. Complete details of this study can be found in the cited pages.

The following reaction equations were considered in the simplified silica-cristobalite-quartz system:

$$\begin{aligned} &SiO_2\,(cristobalite) \leftrightarrow SiO_2\,(aqueous) \\ &SiO_2\,(quartz) \leftrightarrow SiO_2\,(aqueous) \\ &SiO_2\,(amorphous\ silica) \leftrightarrow SiO_2\,(aqueous) \end{aligned} \tag{3-32}$$

where other silica minerals have been neglected. Important features of this system are that solubility of silica increases with temperature and that dissolution rates increase with temperature. The influence of these reactions on the permeability and porosity of fracture and matrix rock are the subject of the referenced analysis. When silica minerals dissolve, possibly in

a condensate zone at elevated temperatures, it is expected that fracture apertures would tend to open up to some degree. Silica-saturated fluids may flow to cooler regions where precipitation will occur, or they can flow to regions where evaporation processes also result in precipitation. At these locations, fracture apertures are expected to close-up to some degree.

The model for reactive transport is written in terms of a first-order reaction-rate equation for silica dissolution and precipitation, conservation of mass for transport of the aqueous phase, conservation of mass for the solid mineral, and a porosity-change equation in terms of the solid mineral phase. For a dual permeability model, the governing equations are written for both fractures and matrix rock. The conservation-of-mass equation for aqueous transport is:

$$\frac{\partial}{\partial t}\phi\rho_l S_l \omega_\gamma + \nabla \cdot \left[\omega_\gamma \mathbf{q}_l - \phi \rho_l S_l \tau_l D_\gamma \nabla \omega_\gamma\right] = -Mr_\gamma \tag{3-33}$$

and conservation of mass for the solid mineral is:

$$\frac{\partial}{\partial t}\rho_\gamma \theta_\gamma = Mr_\gamma \tag{3-34}$$

The resulting porosity change is computed with:

$$\frac{\partial}{\partial t}\phi = -\sum_\gamma \frac{\partial}{\partial t}\theta_\gamma \tag{3-35}$$

where,

ϕ	=	porosity
θ_γ	=	volume fraction of mineral phase
ω_γ	=	mass fraction of aqueous silica
S_l	=	liquid phase saturation
ρ_l	=	liquid phase density (kg/m^3)
$\mathbf{q}_l$	=	liquid phase mass flux (kg/s-m^2)
τ_l	=	liquid phase tortuosity
D_γ	=	diffusion coefficient (m^2/s)
M	=	molecular mass of silica (kg/kmol)
ρ_γ	=	density of the solid mineral (kg/m^3)

The first-order reaction rate equation, r_γ ,is written for (γ =cristobalite, quartz) as a function of a dissolution-precipitation rate constant (different for each process), an equilibrium constant, and the mineral specific surface area. The exact form of the reaction rate equation is given in Hardin (1998, pp. 5-59 and 60). The capillary pressure and intrinsic permeability in the fractures and matrix rock are assumed to scale inversely with porosity (given in Equation [3-35]) and as the cube of the porosity, respectively.

Equations (3-33) through (3-35) are coupled with TH in a sequential manner. The TH equations are solved for a single time-step. The reactive transport equations (given above) are then passed the solutions from the TH step (for example, T, S_l, $\mathbf{q}_l$, ρ_l)potentially at a smaller time step than that used in the TH part. The reactive transport equations are solved until they reach the end of the TH time step. The new porosity field (for example, ϕ)computed by the reactive transport equations is passed back to the TH equations and the process continues.

The results of this process are shown using a DKM for heat and fluid flow. Relative porosity changes are shown for the fractures and matrix for three different mineral surface areas. Silica precipitation in the fractures resulted in a two-orders-of-magnitude reduction in the fracture aperture. Based on the cubic law for flow between parallel plate fractures, this resulted in a reduction in bulk permeability by six orders of magnitude. The precipitate forms above and to the sides of the emplacement drifts. It forms a "cap" of precipitation above and to the sides of the emplacement drifts. There is a slight gas-phase pressurization below the precipitation cap.

The influence of a precipitation cap forming on the conditions inside the emplacement drift is investigated at the waste-package surface. Figure 5-35 in Hardin (1998, pp. 5-64) indicates waste-package response curves with and without silica reactive transport included. From this figure, the waste-package response curves (such as temperature and relative humidity) are different for each case considered; however, the differences are not large enough to cause an appreciable response (if any at all) from the waste package corrosion models used to compute the degradation of the canister. Based on this result, THC effects are neglected for the base-case TH calculations in support of TSPA-VA. Further study is required including consideration of different mineral types.

This study goes on to consider the effects of infiltration and hydrologic parameters on the formation of a precipitation cap. The extent and duration of a precipitation cap surrounding the drift are greatly influenced by the hydrologic parameters. For property sets with high fracture capillarity, the formation of the cap completely encloses the emplacement drift. The influence of the precipitation cap on seepage into the drift requires further future studies. A precipitation cap can affect performance if the cap impedes or enhances seepage flow into emplacement drifts. This is a topic for further study leading into the license application.

3.6.8.3 Near-Field Environment Expert Elicitation

The Near-Field-Environment Expert Elicitation was established because there were large uncertainties associated with THM and THC processes. The panel was specifically tasked with considering how these processes occur, both temporally and spatially, and over what range of values the hydrologic properties (for example, fracture permeability) may be influenced. An

important goal of the Expert Elicitation was to characterize uncertainties associated with coupled effects in the near-field/altered zone.

The elicitation panel examined the most recent project process models as well as experimental data on coupled processes from the single-heater test. They considered THM and THC processes, potential changes to interactions between fractures and matrix rock, and effects of rockfalls, with an emphasis on how rockfalls influence TH conditions in the rubble within a drift. The panel found that fracture-permeability changes may occur in both the vertical and horizontal directions and in condensate and boiling zones. According to the experts, fracture permeability in the vertical direction can either decrease by 10 to 100 times or increase by 10 to as much as 1,000 times, depending on spatial location. Fracture permeability in the horizontal direction may increase by no more than 10 times. Based on the results of the elicitation, the potential for thermally driven alteration of fracture properties (for example, permeability) falls within the range of natural variability because of natural heterogeneity of the system. However, the thermally driven component of fracture alteration may tend to push this range toward the smaller values of fracture permeabilities. The panel concluded that the mechanical effects will tend to be reversible upon cooling, with the possible exception of horizontal changes in permeability resulting from shear stress, but that chemical effects will be more permanent. The panel indicated that the fracture-matrix interaction parameter used in the dual-permeability models may also be affected by chemical precipitation or dissolution processes. This effect may be permanent; however, the range of change for this parameter because of heating processes is uncertain.

The expert-elicitation results and the preliminary modeling studies of THM and THC processes are the bases for not including these coupled-process effects in the TH analyses for the TSPA-VA base case. This assumption requires further study.

The expert panel included the participants given in Table 3-39. The details and the results of the Expert Elicitation are found in (CRWMS M&O 1998, p. 1-6 of 8).

3.6.9 Summary of Sensitivity Studies for Thermal-Hydrology

The TH models exercised for hydrologic property sets other than base case indicated insensitivity of the models to predicted results in the near-field environment as well as gas-phase flow data such as air mass fraction. The "thermal-hydrologic property set" did provide for some extended superheated conditions for repository subregions located near the lower nonlithophysal host units.

Repository design options included consideration of different backfill materials for the reference repository point-load design. The extent of relative-humidity reduction is greatly enhanced for backfill cases. Backfill also obviates the need to consider a rockfall-rubble scenario. As shown in the rockfall study, the relative humidity initially decreases but then increases to a level even higher than for an open emplacement drift. In the sensitivity study, rockfall occurred at 1,000 years after waste emplacement. If rockfall happens to occur sooner after waste emplacement, the increase in relative humidity in the rockfall zone surrounding the waste package may be very detrimental to performance of the waste package.

Different repository designs were also considered in the section. For the case of a line-load repository design with a quartz-sand backfill, the relative humidity reduction was seen to persist for tens of thousands of years. (This is a positive feature with respect to waste-package performance.) Future consideration of the line-load design would require a change in philosophy by the project. Its relative merits (relative-humidity reductions) and drawbacks (specific backfill procedures such as no backfill between close packages) have been set forth. Waste-package sequencing was also considered at the scale of the drift. Hotter and colder than average drift segments indicate differences in waste-package response curves at early times only. After thousands of years, the drift segments behave in a very similar manner. A final sensitivity study that seems to indicate a substantial deviation from the base case is for a TH model for open drifts (i.e., an emplacement drift with a continual source of air during the heat decay process). This is a scenario not unlike a ventilated repository. The sensitivity of air mass fraction and gas-phase mass flux is quite sensitive to this feature. Drift-scale calculations did not consider this feature, so it is unclear how the waste packages would respond to such a process (open drifts with a continual source of air). The implications to performance and guidance for the license application are the subjects of the next section.

3.7 SUMMARY AND RECOMMENDATIONS

There are no system-level sensitivity analyses related strictly to TH for the TSPA-VA. The most important TH issues considered are related to hydrology (hydrologic parameters, fracture-matrix interaction, and infiltration rates) and repository design (backfill, thermal load, and waste-package spacing). Issues related to hydrologic parameters and fracture-matrix interaction are discussed in Chapter 2 of the TSPA-VA Technical Basis Document on UZ flow. The TH implications of hydrologic issues (climate change, infiltration uncertainty, hydrologic-property uncertainty, and alternative flow models) were considered. In fact, they are incorporated in the UZ flow sensitivity analyses where lower temperatures related to high infiltration rates are shown to have a strong effect on doses for approximately the first 20,000 years. Some variations in repository design were considered as well, including emplacement of backfill 100 years after emplacement of waste. Analyses of alternative designs and other sensitivities were discussed in Section 3.6.

Other potentially important issues—THC and THM processes and effects—are largely left to future work. They may be important, and they need to be evaluated more fully. In a simplified analysis, THC and THM sensitivity studies described in Section 3.6 indicate that the impact of these processes does not drastically influence the results of the base case models applied to TH. This requires further consideration.

3.7.1 Implications for Performance

A key attribute of the repository safety strategy is limiting water contacting waste packages. This includes factors such as infiltration, seepage into drifts, humidity, and temperature at waste packages, and dripping onto waste packages. Infiltration and humidity and temperature at the waste packages are considered in detail in Sections 3.5 and 3.6. Seepage into drifts (nonisothermal) is considered as a sensitivity study in Section 3.6. The importance of each to performace are discussed as the following.

It was shown in Section 3.5.5 that infiltration rate influences computed repository temperatures. Within the range of infiltration uncertainty incorporated in the TSPA-VA base case, the changes in temperature are not large, but as shown in the sensitivity studies for UZ flow, they can still have a significant effect on computed dose rates during about the first 20,000 years. For high infiltration rates, temperatures in the repository are lower and hence dose rates are higher. Therefore, for TH as well as for other TSPA-VA components, characterization of current and future infiltration is important.

The TH uncertainty, characterized by a property set with reduced fracture capillarity in the host units as well as reduced, matrix-imbibition diffusivity in the lower host units, can be shown to reduce the dose rate (in mrem/year) by more than an order of magnitude (compared to the base case) in repository subregion SW for the 10,000 year expected-value dose-rate history. Subregion SW repository horizon is in the lowermost host unit (the lower nonlithophysal unit). With the reduction in fracture and matrix capillarity, the rate of rewetting is reduced and superheated regions (near the SW) can persist longer. This is seen to have a positive impact on the repository performance (near the southwest corner). In other subregions away from the southwest corner of the repository the impact is not as dramatic. The dose rates are very similar (although slightly less) to those computed with the base-case property set. For expected-value dose-rate histories out to 100,000 and 1,000,000 years the difference in property sets is negligible. Therefore, this effect is important only for a 10,000-year calculation and only near the southwest portion of the repository.

Temperature and relative humidity are seen to vary appreciably for different design options, but not for different property sets for a given design. The impact of temperature and relative humidity and repository performance rests on the lifetime of the waste package. Thermal reflux will also play a part in determination of the waste package lifetime. Thermal reflux is that water driven by repository heat. The appropriate characterization of thermal reflux is strongly dependent on conceptual flow model. It impacts the relative humidity, temperature, and seepage into drifts during the heating period. With the exception of the nonisothermal seepage study into drifts given in Section 3.6, drift seepage considerations include infiltrating water only. Fortunately this is adequate for late times when most waste packages fail. It does not include how THC may have altered flow properties around the drifts at late times. The impact of this neglected process and how it influences performance is not known. These are topics for future consideration and discussion in the next section.

3.7.2 License Application Guidance for Thermal-Hydrologic Models and Testing

As mentioned above, there are two categories of potential improvements to future TH models. One category is improved characterization of the hydrology, including infiltration rates, fracture and matrix hydrologic properties, and fracture-matrix interaction. The other category is improved incorporation of mechanical and chemical coupled processes. Finally, a discussion is given of how heater tests have and will be applied to this and future TSPAs.

3.7.2.1 Properties

The variations in hydrologic properties and alternative conceptual flow models investigated for the TSPA-VA did not produce any significant effects on computed repository performance,

although significant differences were found between results using the DKM and the ECM. The DKM allows for greater mobility of water in fractures, which has a great effect on modeled condensate buildup and drainage. A related flow issue that could be important to TH is channelized flow, especially in discrete fractures. Such flow could greatly increase the spatial variability in the results by increasing the range of water-flow rates seen by individual waste packages. Therefore, effects of such concentrations of flow should be investigated.

There is some concern about lack of imbibition-based hydrologic properties for the rock matrix. Almost all of the available data on matrix hydrologic properties have been obtained from drying experiments. For modeling the TH behavior during rewetting and condensate drainage, data obtained from both wetting and drying experiments would be more appropriate. Wetting and drying properties can be very different because of hysteresis. The "thermal-hydrologic property set" mentioned in Section 3.6.2 was intended as a better representation of wetting hydrologic properties. While the TSPA results for the TH property set are not significantly different from the base-case results, obtaining more imbibition data would ensure that the project has the appropriate matrix hydrologic properties.

3.7.2.2 Thermal-Hydrologic Experiments

The primary source of new information for improving TH models will be the Drift Scale Test already underway at the Exploratory Studies Facility. The results of the early heating period of this large-scale test will be available in time for the TSPA for the license application. This test will provide information on drift-scale movement of heat through rock at Yucca Mountain and its impact on the flow system above and below an emplacement-sized drift. It will include a detailed investigation of the heating period and movement of heat-driven water as well as the cooling period and subsequent rewetting analogous to the processes that would occur in the repository. Indirect measurements to detect water flow into the drift during heating will provide crucial information related to thermal refluxing processes driven by larger-scale heat-transfer processes. The data obtained from the heated-drift test will

- Allow important verification of the conceptual flow models currently being used (or show the degree to which the current models are not adequate)
- Provide information on the effective hydrologic properties during the various stages of heating and cooling
- Provide information on the spatial and temporal extent of mechanical and chemical changes to the fracture-flow system surrounding the heated drift.

Smaller scale tests include the already completed SHT at the Exploratory Studies Facility or any other future single- or multiple-element heater tests that may be planned for the East-West cross drift to be constructed in the near future. This experimental scale provides an excellent opportunity for conceptual-flow model validation. In fact, this has already proven useful in determination of an appropriate flow model used to predict heat-driven processes that governed the results of the SHT. Initial results from the SHT seem to indicate that the DKM is most appropriate in governing heat transfer and fluid-flow processes and subsequent temperature field predictions. This knowledge has already proven very useful for TSPA-VA in that it guided

project decisions in selecting the hydrologic property sets required to generate the flow fields that govern the rate at which radionuclides travel through the UZ. To date, we have successfully tested conceptual flow models and hydrologic property sets against actual heating and cooling data for a heater test carried out in one of the repository host rock units (Topopah Springs Middle Nonlithophysal). We have, based on actual experimental data, made assessments regarding conceptual flow models that should be applied in the TH analyses used in support of this TSPA and future TSPAs used in the license application.

In order that the project further refine the flow-field predictions used in the TSPA transport calculations, future heater tests, carried out in the other two repository host units (Topopah Springs Lower Lithophysal and the Lower Nonlithophysal), must be considered. The heater tests can either be single element or planar heat source in nature. Future testing would provide more valuable information related to hydrologic properties and more importantly to the conceptual flow models that should be applied to the units in which the repository will be directly placed. Future small-scale tests will then lend credence to the TH models that are used to predict heat and fluid flow processes in repository-scale calculations over much longer periods of time.

3.7.2.3 Coupled Processes

The greatest potential shortcoming of the TSPA-VA TH calculations is the lack of coupling to thermal-mechanical and thermal-chemical processes. These issues have been addressed to a limited extent (see Section 3.6), but the full range of possible (or even likely) behaviors has not been analyzed. The Near-Field-Environment Expert Elicitation will aid in considering these issues, but it was not completed until after the TSPA-VA analyses were finished. Therefore, implementing the recommendations from the expert elicitation remains to be done.

Future studies will also require investigation of coupled processes driven by the thermal load. This can be experimental in nature or from process-level modeling analyses. Indeed, the large-scale, heated drift-scale test should provide useful data related to THM processes as well as THC processes. This includes discovery of alterations (if any) to the fracture system surrounding the heated emplacement drift by thermal stresses and/or dissolution-precipitation processes. Indications of these coupled processes including alterations to fractures, can also be surmised from the smaller scale tests as well. This has already been done for the SHT with respect to mechanical displacements and post-test analyses of water chemistry and can be done for any future tests planned in the other repository host rock units. Future modeling studies will also play an important role in reducing the uncertainties associated with coupled processes.

Drift-scale THC analyses for silica or calcite dissolution-precipitation processes will be required to assess chemical alteration in the fractures near the heat sources emplaced into the UZ. This reactive transport process can either increase or decrease fracture porosity and permeability as minerals move from regions where condensate waters flow. At the scale of the drift, heat transfer from the waste packages to the drift wall will drive evaporation processes in the rock that will leave mineral deposits in the fractures where fluids flow.

Mineral caps that may form could create a resistance to flow in one direction which could result in the formation of new flow-paths for water moving into or around the emplacement drifts.

These chemical processes may result in a permanent alteration in the flow paths (i.e, chemically altered zones that persist beyond the thermal periods of the repository heat output).

A chemically altered mineral cap surrounding the emplacement drift has been found to form as a result of phase-change processes during thermal loading applied to modeling studies and as investigated in natural analogs. Preliminary modeling studies (Hardin 1998, pp.5-57 through 5-67) of a silica system have indicated the formation of a mineral cap directly above the emplacement drifts. Depending on the imbibition characteristics of the hydrologic properties applied to the host rock, the cap may close in on the sides of the drift as well as in between emplacement drift pillars. Comparisons to natural analogs (the Papoose Lake Sill, W. Matyskiela 1997) also seem to indicate that heating of fracture fluids may cause depositions of minerals that can serve to alter the flow through the fracture system surrounding the heat source. An assessment of the chemical alteration to the physical processes governing the water flow characteristics between fracture and matrix rock has also been given in this natural analog study. As indicated by the expert panel in the Near-Field Expert Elicitation the "interaction" parameter is potentially a key factor in describing the processes altered by chemistry and subsequently the manner in which fractures and matrix rock communicate with each other. This "process" requires further sensitivity studies with TH process-level models that include both the dual permeability formulation as well as the reactive transport equations. Although the comparison of this natural analog to the repository may be fair in many respects concerning chemistry alterations to the fracture flow paths, the power output of the sill described in this study is much higher than that of the repository. Therefore, the temperatures in the rock surrounding the sill will be much higher than the host-rock temperatures surrounding the emplacement drifts of the potential repository. The importance of this investigation is not lost however, so that process-level modeling of chemical alterations to fracture properties must be considered in the license application time frame.

Future modeling studies using appropriate conceptual flow models must be performed for THC processes occurring at the scale of the drift. It is essential that the flow processes by accurately represented so that an assessment can be made as to whether or not the development of mineral deposits is physically realistic. That is, will the water remain in the system long enough to allow for deposits or will it flow through the fracture network during the condensate drainage period so that evaporation will not occur to the bulk of the fracture waters and precipitation in fractures is minimal. All of the effects related to chemistry alteration have been neglected for the current TSPA. That is, the TH is uncoupled from the chemistry. This is also the case for mechanical processes driven by repository heating.

Although not as enduring as the chemistry-driven processes, THM processes may alter fracture properties so that the flow fields may be altered during processes of thermal expansion and compression during the heating period of the TH models. Most of the mechanical effects tend to be reversible, with the possible exception of shear slip on the horizontal fracture network. However, based on the results of the expert panel review, this would result in, at most, a potential permanent permeability change of up to ten times the natural value. The mechanical influence on the fracture network may require further analysis with respect to large-scale gas-phase flow effects driven by the thermal load while the repository is at its hottest. If fracture flow properties are changed so that porosity and permeability are reduced, heat and mass movement away from the repository horizon in the form of convection may be restricted. This

may result in temperature or pressure changes at the repository horizon, thus altering mountain-scale TH predictions (air mass fraction, gas-phase flux) used in the near-field geochemical models.

3.7.2.4 Repository Design

Potentially important future natural-system studies have been documented and considered in some detail in the preceding paragraphs. Future considerations or changes made to TH models must also incorporate any design options or engineered enhancements that may be considered by the repository designers. This includes placement of flow barriers or other engineered approaches used to mitigate the movement of liquid water or provide for reduced relative humidity in the vicinity of the waste packages.

Thermal-hydrologic analyses for the total system viability assessment included placement of a crushed-tuff and quartz-sand backfill. The emplacement drift is partially filled with a low thermal conductivity material in direct contact with the waste packages 100 years after onset of waste loading. This option (refer to Section 3.6.3) provides for longer periods of relative-humidity reduction in the environment surrounding the waste packages. It also leads to higher waste-package surface temperatures. Because high temperatures are associated with a low thermal conductivity fill, the environment surrounding the waste package remains hot and dry for a longer period of time than does the reference-repository design for an open drift. An assumption applied to the backfill analyses in this document is that the fill material is emplaced "bone dry." If this is not the case, that is, the matrix rock of the fill does contain some initial water, evaporation will occur directly at the surface of the waste package during the early heat-up period. The surrounding environment will still be very hot so that completely dry conditions can be attained. However, in this case, evaporation occurs at the surface of the waste package instead of at the drift wall. In this scenario, it is possible that solids will precipitate out of the water and directly onto the waste-package surface. It may be necessary to consider future modeling studies that include placement of a "wet" backfill to determine the time required to boil the water in order to make an assessment as to the corrosive potential at early times of this design option. Other heat-control options may be centered on forced-air convection through the drifts.

Potential design options that include an extended period of ventilation (100 years or more) before repository closure must also be considered by performance assessments to determine the impact of such ventilation on post-closure repository performance. An extended period of ventilation has the effect of aging the waste for an extended period of time. This is a direct result of forced-convection cooling (by forced airflow through the emplacement drifts) of the waste emplaced in the repository during the extended pre-closure period so that emplacement drift and waste package temperatures remain low. If an extended period of ventilation is specified, then all wastes, not just the waste loaded early on, will have an extended time period in which to cool. Performance assessments will require thermal-hydrologic models that include waste stream variability (mountain-scale and drift-scale) with waste packages and a total waste inventory that is cooler than the instantaneous emplacement of all wastes without thermal decay. Also, after repository closure, ventilation air flow will have removed water from the emplacement drift walls such that the energy requirement needed to vaporize in situ water (near the drifts) is removed and the energy imparted to the rock (that is already dried) goes directly into raising the temperature of the host rock. This may impact the predicted engineered barrier performance, and

the thermodynamic environment within the drift after permanent closure. As an example, the resulting impact of ventilation processes on repository heating may be analogous to the "cold" emplacement drift segment analysis presented in Section 3.6.4 with some of the latent heat requirement removed by initial evaporation driven by ventilation. In the case of extended ventilation (as in the case of the cold drift segment), the emplacement drift *kW/meter* will effectively be reduced at the time of final closure. This will effectively result in less time above boiling, with increased relative humidity in the emplacement drifts at late times. The continued formation of a dryout zone around the drifts will be smaller as less heat will be available for vaporization and subsequent vapor movement outward.

In the TSPA-VA TH base-case analyses, it is assumed that the waste is simultaneously emplaced at repository closure (Section 3.6.4 considered a delayed thermal-loading case). In this scenario, waste-container heat outputs are a maximum. For the base-case waste stream, this results in the greatest availability of heat for temperature increases with subsequent dryout formation and relative-humidity reduction and the potential for heat-mobilized waters to move through the cooler pillars between emplacement drifts. The impact of this assumption compared to a ventilated (for extended periods) design option must be assessed with respect to long term repository performance.

Each of the options set forth by the repository design team need to be considered in any total system performance assessment calculation in order to determine the design impacts on long-term performance of the potential repository. Future considerations of design options or enhancements will need to be closely coordinated with PA and the appropriate design groups.

Guidance for the license application with respect to TH includes both natural system and design option considerations. Coupled processes, including experimental and process-level modeling investigations of the heating impact on system hydrology, chemistry, and mechanics, largely drive natural-system considerations. Other important issues regarding design options or other engineered enhancements to the repository reference design must be closely coordinated with the performance assessment group so that potential impacts may be assessed with respect to long-term performance of a potential geologic repository at Yucca Mountain.

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