5. EFFECTS OF DECAY HEAT ON IN-DRIFT THERMAL-HYDROLOGIC CONDITIONS

This section discusses model development and analyses conducted since completion of the *Yucca Mountain Science and Engineering Report* (S&ER) (DOE 2001 [DIRS 153849]), in the area of thermal-hydrologic (TH) influences on in-drift conditions. The section begins with a short review of the conceptual basis for TH modeling of the in-drift environment. The review is followed by a summary of the treatment of thermal hydrology in *Total System Performance Assessment for the Site Recommendation* (TSPA-SR) (CRWMS M&O 2000 [DIRS 153246]), which is the model that supports the S&ER. The purpose of this section is to document the improvements that have been made to the TH process model and its abstraction for total-system modeling since completion of the TSPA-SR. The model revisions and analyses were conducted to improve the implementation of the scientific conceptual model, quantify previously unquantified uncertainties, and evaluate how a lower-temperature operating mode (LTOM) would affect the in-drift TH environment, as summarized in Table 5-1.

The improved model was exercised at the process-level and the total system-level for this report. Section 5.1 introduces the conceptual basis upon which the model is based. Section 5.2 reviews how the in-drift TH environment was modeled in support of the TSPA-SR and S&ER. Section 5.3 describes uncertainties in the models, improvements in the models to reduce those uncertainties, and analyses conducted to better understand them. This section (5.3) is split into two parallel subsections addressing the multiscale TH modeling of in-drift conditions and modeling of ventilation and convection. These sections are followed by another section (Section 5.3.3) summarizing the available natural and anthropogenic analogue information applicable to in-drift TH conditions. Each of the two parallel sections (Sections 5.3.1 and 5.3.2) includes a discussion of process model goals, representation in TSPA-SR (CRWMS M&O 2000 [DIRS 153246]), subsequent model improvements, and quantification of uncertainty using the improved model. The two parallel subsections include 17 discussions of individual aspects of uncertainty. For convenience, each of these discussions includes a short summary, and there is an overall summary of the 17 analyses in Section 5.4.3.

The final section (Section 5.4) of the chapter discusses the results of the exercise of the multiscale TH model in support of the SSPA Volume 2 (McNeish 2001 [DIRS 155023]) base case higher-temperature operating mode (HTOM) and LTOM. It also provides an overall summary of results of the process model-level results that quantified uncertainty.

5.1 INTRODUCTION AND CONCEPTUAL BASIS

The heat produced by radioactive decay of the nuclear waste in the potential repository will have an effect on the seepage water into the potential repository drifts, water movement through the potential repository, and the patterns of natural water flow in the unsaturated rock layers which set the boundary conditions for the in-drift environment. The nature and extent of these effects, however, will depend on thermal loading (or areal heat output), ventilation rates and durations, and consequent operating temperature mode (i.e., above-boiling or below-boiling). The goals of the process-level and total system performance modeling of the effects of decay heat on in-drift thermal-hydrologic conditions are to develop estimates for the evolution of key environmental conditions in the emplacement drifts. These models must consider the effects of heat on water

Table 5-1. Summary of Supplemental Models and Analyses

Key Attributes of System	Process Model (Section of S&ER)	Topic Of Supplemental Scientific Model or Analysis	Reason For Supplemental Scientific Model or Analysis			Performance Assessment Treatment of Supplemental Scientific Model or Analysis[a]		
			Unquantified Uncertainty Analysis	**Update in Scientific Information**	**Lower-Temperature Operating Mode Analysis**	**Section of Volume 1**	**TSPA Sensitivity Analysis**	**Included in Supplemental TSPA Model**
Long-Lived Waste Package and Drip Shield	Water Diversion Performance of EBS (4.2.3)	Multiscale thermal-hydrologic model, including effects of rock dryout	X		X	5.3.1		X
		Thermal property sets	X	X		5.3.1		X
		Effect of in-drift convection on temperatures, humidities, invert saturations, and evaporation rates	X		X	5.3.2		
	In-Drift Moisture Distribution (4.2.5)	Environment on surface of drip shields and waste packages	X			5.3.2		
		Evaporation of seepage	X		X	5.3.2	X	X

NOTE: S&ER = *Yucca Mountain Science and Engineering Report* (DOE 2001 [DIRS 153849]).

[a] Performance assessment treatment of supplemental scientific model or analysis discussed in SSPA Volume 2 (McNeish 2001 [DIRS 155023]).

movement in the host rock near emplacement drifts; however, this section reports only the results for TH conditions within the drift or at the drift wall. Key parameters contributing to the environmental conditions in the emplacement drifts include temperature, relative humidity, and evaporation rates that affect the performance of the engineered barriers and the transport of radionuclides that may eventually be released.

The major effects of decay heat on water movement that could impact the in-drift conditions would occur immediately after permanent closure (DOE 2001 [DIRS 153849], Section 4.2.2), at which time the ventilation system is shut down. Initially, heat will be transported outward away from the drifts by heat conduction through the rock and the movement of air through fractures. A portion of the heat will be transported by water that vaporizes near the heat sources and condenses in cooler rock farther away. If the heat flux (from the waste package resulting from decay of the waste) is high enough, rock near the drifts will be heated to the boiling point of water (nominally 96°C [205°F] at the elevation of the potential repository), and then to higher temperatures after most of the water in this region has evaporated. How the rock responds (dryout/rewetting) will impact the conditions within the drift. The time during which rock drying and wetting occurs, and thus impacts the in-drift conditions will depend on local thermal loading, percolation flux, and location in the potential repository layout (i.e., near the center or the edge). As the heat produced by radioactive heat declines with time, temperature within the emplacement drifts will return to pre-emplacement levels.

Thermally-driven processes are most intense within, and in the immediate vicinity of, the emplacement drifts. However, larger-scale processes (mountain scale) must be considered as well because they affect the drift environments. Thermal processes at the drift scale (a few meters to tens of meters, or several feet to several tens of feet) include conduction within the rock and the radiant heat transfer within the drifts. To these are added all the processes associated with liquid and gas flow including thermal effects due to evaporation and conduction. Additional important considerations at the mountain scale (hundreds of meters to thousands of meters, or several hundred feet to several thousand feet) include the surface topography, the stratigraphy of the unsaturated zone, and the spatial variations in infiltration. Surface topography refers to the thickness of the overburden above the emplacement drifts and is a factor in how quickly a location cools off. The stratigraphy of the unsaturated zone influences the thermal and hydrologic properties of this zone that can be quite different across stratigraphic units. The spatial variation of thermally-driven processes indicate that higher infiltration leads to lower temperature and higher relative humidity, and faster cooling of the potential repository edge as compared with its center.

Consistent with the *Unsaturated Zone Flow and Transport Model Process Model Report* (CRWMS M&O 2000 [DIRS 151940], Section 3.10.3.1), the engineered barrier system thermal hydrologic models use the dual-permeability conceptual flow model to characterize the flow of heat and moisture through the rock of the potential repository. The flow of heat and moisture are modeled as flowing through two interacting continua, with each continuum being assigned its own spatially variable hydrologic properties, such as permeability and porosity. Fracture-matrix interaction is represented with an active-fracture model, in which only a portion of the fractures are actively flowing under unsaturated conditions (CRWMS M&O 2000 [DIRS 151940], Section 3.3.4).

Drift-scale modeling must include coupling of drift-scale processes with mountain-scale processes to properly account for effects such as faster cooling of waste packages near the potential repository edge, as compared to waste packages near the potential repository center. Because of scale issues, directly modeling the evolution of in-drift thermal hydrology in detail and in three dimensions would require extreme levels of computational effort. To alleviate this problem, a multiscale model, called the *Multiscale Thermohydrologic Model* report (CRWMS M&O 2000 [DIRS 149862]) (MSTH model), was developed that combines submodels that consider the scale of interest for a particular portion of the problem. The validation of the MSTH model, as discussed in Section 5.3.1.2.1, relies on comparison between model results and field studies designed to test the validity of the model. This comparison is reported in the *Multiscale Thermohydrologic Model* report (CRWMS M&O 2000 [DIRS 149862], Section 6.13.2). That document reports good agreement between the model and the measurements made in the Drift Scale Test. The Drift Scale Test was designed to test the coupled process models, including the MSTH model, and is being conducted underground in the environment appropriate for testing these models.

The multiscale approach also breaks the problem into more tractable pieces by considering dimensionality requirements (one-, two- or three-dimensional) for the issue of concern. For example, considerations of mid-pillar temperatures may be appropriately modeled with two-dimensional calculations, but temperature distributions within a drift with varying package outputs requires a three-dimensional calculation because temperatures vary in three dimensions. The multiscale approach divides the problem into thermal and thermal-hydrologic submodels so that the effects of convective heat transfer and phase change of water in the rock, in addition to conduction can be addressed efficiently. By dividing the problem into a more efficient conduction submodel can be used to address detailed three-dimensional problems where that submodel is sufficient, such as when there is no moisture present or when there are no effective pathways for moisture movement. When conduction submodels are not sufficient, a convective heat transfer submodel can be applied, but without considering as much three-dimensional detail. By combining these in a MSTH model, both heat and mass transfer can be efficiently evaluated.

A major strength of the MSTH model is that it precisely represents the influence of many details of potential repository design on the predicted thermal-hydrologic responses throughout the potential repository volume. This means that the MSTH model results are design-specific and that the use of different design parameters would potentially yield different results. However, the results may be considered to be approximately applicable to alternative designs that share similar dependent-parameter attributes, such as peak temperatures and that share similar design attributes, such as waste package spacing. In the *Multiscale Thermohydrologic Model* report (CRWMS M&O 2000 [DIRS 149862]), thermal-hydrologic responses were analyzed for a case in which boiling temperatures extend a short distance (< 10 m for the mean infiltration-flux scenario) into the rock. This is the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) design case.

For the SSPA, two cases were analyzed using the MSTH model (BSC 2001 [DIRS 154864]). The first case analyzed, called the HTOM, is similar to the TSPA-SR design case, but analyzed with updated models. Operating the potential repository at lower temperatures would reduce the magnitude and duration of the effects of decay heat on water movement. In addition, lower temperatures would result in reduced chemical reaction rates so that the effects of the coupled

THC processes would also be reduced, as discussed in the *Drift-Scale Coupled Processes (DST and THC Seepage) Models* (BSC 2001 [DIRS 154677]). The second case analyzed, called the LTOM, is one where temperatures do not exceed approximately 85°C on the waste package surface. These potential repository conditions are achieved in the model analyses that were conducted using the specific operational-mode assumptions listed in Table 5.1-1. If corrosion testing and modeling for the SSPA and a potential license application conclude that localized corrosion in the 85°C to boiling temperature range is not likely for potential repository chemical conditions, then the intermediate case could be analyzed.

5.2 REVIEW OF TOTAL SYSTEM PERFORMANCE ASSESSMENT-SITE RECOMMENDATION TREATMENT

The in-drift TH environments for TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) simulations were computed using the MSTH model (CRWMS M&O 2000 [DIRS 149862], Section 6.1). This AMR included modeling of the no-backfill scenario, providing temperature and relative humidity at several in-drift locations, and liquid evaporation rate and saturation values in the drift invert gravel. Because the processes couple beyond the drift wall, the MSTH model calculates conditions within the rock in order to accurately reflect the development of TH conditions within the drifts. Thus, in addition to in-drift uses of these results, the MSTH model provided information regarding near-field water flow rates to the thermal seepage model. Although the information provided by the analysis of the thermal hydrology to other TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) model components, and inputs from other TSPA components to the analysis of thermal hydrology, are summarized in Figure 5.2-1, this section focuses on the in-drift processes. A multiscale modeling and abstraction method was developed to couple drift-scale processes with mountain-scale processes. This method uses a series of submodels, one mountain-scale and three drift-scale submodels, to abstract the thermal hydrologic quantities throughout the potential repository area (Figure 5.2-2). The four submodels are described briefly below. Additional details are included in the *Multiscale Thermohydrologic Model* (CRWMS M&O 2000 [DIRS 149862]).

Line-Averaged-Heat-Source, Drift-Scale, Thermal-Hydrologic Submodel–The line-averaged-heat-source, Drift-Scale, Thermal-Hydrologic (LDTH) submodel is a two-dimensional drift-scale (chimney) model that computes temperature and moisture-related quantities (relative humidity, liquid saturation, liquid flow rate or flux, and liquid evaporation rate) at several locations within and near the drift. This submodel effectively represents average thermal hydrologic behavior at any specific location within the potential repository, taking into account the location-specific thermal and hydrologic properties, boundary conditions, and percolation flux. The (LDTH) submodels use the dual-permeability method (DKM), modified with the active fracture concept (AFC) for fluid flow in the fractured porous rock. The DKM conceptualizes the fractured rock as having two interacting materials, one representing the matrix and one representing the fractures (CRWMS M&O 2000 [DIRS 149862], Section 6.3). The AFC accounts for the contact area between the fracture and the matrix, as well as the frequency of fractures. The AFC means that the fracture flow only occurs through some of the fractures. Within the drift, thermal radiative heat transfer is explicitly represented and natural-convective heat transfer is represented using an effective thermal conductivity of the air occupying the space between the drip shield and the drift wall (CRWMS M&O 2000 [DIRS 153246]).

Smeared-Heat-Source, Mountain-Scale, Thermal-Conduction Submodel–The smeared-heat-source, mountain-scale, thermal-conduction (SMT) submodel is a three-dimensional model that includes the stratigraphy, topography, and layout of the potential repository considering only thermal-conduction heat transfer. It is used to determine the repository-scale variations in host-rock temperature resulting from the total heat output and includes the influence of the potential repository edges, the topography, and the mountain-scale variability in stratigraphy and thermal properties of the geologic units.

Smeared-Heat-Source, Drift-Scale, Thermal-Conduction Submodel–The smeared-heat-source, drift-scale, thermal-conduction (SDT) submodel is a one-dimensional model that considers only thermal-conduction heat transfer. It is used to establish temperature relationships and to account for the influence of repository edges, topography, and mountain-scale variability in stratigraphy and thermal properties of the geologic units.

Discrete-Heat-Source, Drift-Scale, Thermal-Conduction Submodel–The discrete-heat-source, drift-scale, thermal-conduction (DDT) submodel includes conductive heat transfer, plus radiant heat transfer within open drifts. This submodel is a three-dimensional model of a drift segment containing representative waste package types and heat outputs representative of the overall potential repository. The scale of the submodel includes a drift segment of sufficient extent to include six waste packages plus two halves (the half-waste packages are on symmetry boundaries). This submodel provides information on the package-to-package heat-output variability along the drift. The model drift segment contains waste.

It is useful to think of the LDTH submodel as the core submodel. The LDTH submodel is run for multiple locations spaced throughout the potential repository area. The remaining three submodels, which are conduction-only submodels (SMT, SDT, DDT), are required to account for the influence of three-dimensional mountain and drift-scale heat flow on drift-scale TH behavior. The MSTH model addresses differences between the potential repository center and edge locations by coupling the SDT submodel with the SMT submodel. The coupling uses the average temperatures of the potential repository host rock obtained from the SMT submodel. The resulting temperatures inherently include the repository edge effects, because they originated from the SMT submodel. The abstracted average results were modified to reflect package-specific temperatures calculated by the DDT submodel.

The MSTH model relates the results from the submodels to capture the effects of key factors that can affect TH conditions in the emplacement drifts and surrounding rock (drift wall):

- Variability of the percolation flux on the scale of the potential repository footprint
- Temporal variability of percolation flux (as influenced by climate change)
- Uncertainty in percolation flux (as represented by the mean, high, and low infiltration flux conditions described in Section 3.3.2)
- Variability in hydrologic properties (e.g., those properties which control fracture-matrix interaction and capillary in fractures) on the scale of the potential repository footprint

- Edge-cooling effect (cooling increases with proximity to the edge of the potential repository)

- Dimensions and properties of the engineered barrier system components, such as the drip shield and invert

- Waste package-to-waste package variability in heat-generation rate

- Variability in overburden thickness on the scale of the potential repository footprint

- Variability in rock thermal conductivity (emphasizing the host-rock units) on the scale of the potential repository footprint.

The MSTH model involves drift-scale calculations at a number of potential repository locations to capture effects and variability of properties and flux. A set of calculations for a given case involved only one computer run using the SMT submodel and only one computer run using the DDT submodel. However, the LDTH submodel and the SDT submodel were run for 31 locations within the potential repository and for five areal mass loadings (to represent edge effects). The results of these 155 submodel runs were interpolated over the potential repository area as a function of local heating conditions to provide a continuous distribution of the thermal hydrologic variables throughout the potential repository area. To model the preclosure ventilation period, the number of model runs was doubled (one pertains to the pre-closure period and the other pertains to the post-closure period), but these additional runs were for a shorter time period (CRWMS M&O 2000 [DIRS 149862], Section 6.6.1). Ventilation was modeled using a waste package design criteria heat output of 70 percent, as stated in the *Ventilation Model* (CRWMS M&O 2000 [DIRS 120903], Section 6.1), for 50 years. Ventilation is expected to dry out the drifts and the surrounding rock because dry air from the surface would be circulated through the drifts. However, this drying was neglected in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]), which is conservative in the sense that more moisture is left in the model, thus lowering the overall heat removal results. The assessment of conservatism is at a high level. More detailed consideration of the effects of ventilation could change that conclusion. For example, ventilation-caused-drying (which is neglected in the base case, but quantified in sensitivity analyses in this section) decreases local thermal conductivity, and hence elevates in-drift temperatures. The preliminary judgement implied by the statement that neglect of drying is conservative is that the temperature increase due to neglect of latent heat removal in the waste stream is larger than the increase due to local depression of thermal conductivity, and that higher temperatures lead to higher dose rates or higher uncertainties in dose rate.

The abstracted temperature, relative humidity, and other quantities were developed for an array of 610 locations in the potential repository (by interpolation among the 31 LDTH and SDT locations) and the two waste package types, Commercial Spent Nuclear Fuel (CSNF) and DOE high-level radioactive waste (DHLW). The 610 locations are shown in Figure 5.2-3.

There were eight different waste packages considered at each of the 610 locations, which resulted in 4,880 individual environment histories. These histories were abstracted into 30 groups for waste package corrosion, radionuclide release, and EBS transport calculations. The same TH results were determined for all three infiltration-flux cases (mean, high, and low flux scenarios) in the TSPA-SR model. Thus, the TH results were combined into ten distinct groups: five infiltration bins (bins are category groups based on varying infiltration rates) for each of the two waste types. However, because of the importance of the variability in waste package failure time, the full suite of 1,220 sets of results (610 locations times two waste types) were provided as input to the waste package and drip shield degradation models. The TH information provided as input to the various EBS models is summarized in Figure 5.2-1, and the parameters that were provided as bin averages are identified. Where bin averaging was not noted in TSPA-SR (CRWMS M&O 2000 [DIRS 153246], Figure 3.3-7), the full set of spatial locations were identified. A complete list of EBS and near-field environment (NFE) variables calculated with the MSTH model at 610 locations are provided in Table 5.2-1.

The procedures used for averaging the various thermal-hydrologic quantities over the infiltration bins are described in detail in *Abstraction of NFE Drift Thermodynamic Environment and Percolation Flux* (CRWMS M&O 2001 [DIRS 154594]). There is one case where the thermal hydrology abstraction does not simply average information from the MSTH model and that is in the determination of the evaporation rate of water at the top of the drip shield. As discussed in Section 7.3.1 of this document, one of the parameters used for the in-drift chemical environment abstraction is the ratio of water evaporation rate to water in flow rate. The MSTH model can calculate these quantities only in a porous medium, which is not the situation at the top of the drip shield. The seepage flow rate at the top of the drip shield is taken from the seepage abstraction (Section 4.3.1), and the evaporation rate is bounded by the amount of heat available to vaporize water on the upper portion of the drip shield. These bounding values are used to estimate how much water could be evaporated by the waste package heat output at any given time (CRWMS M&O 2001 [DIRS 154594], Section 6.3.10).

5.2.1 Overview of Total System Performance Assessment-Site Recommendation Thermal-Hydrologic Results

Calculations indicate that the heat generation rate from radioactive decay decreases rapidly with age of waste for a period of time followed by slowly decreasing levels for thousands of years. The initial heat output and its rate of decrease with time depend upon the type of nuclear waste. Calculations indicate that the potential repository characterized in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) would initially produce approximately 80 MW of thermal power (BSC 2001 [DIRS 155107], Section 2). The thermal power output will decrease to approximately 25 percent in 100 years, 12 percent in 300 years, and 2 percent of its initial value in 10,000 years.

For the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) design, a requirement was imposed that continuous forced ventilation of emplacement drifts during operations would remove at least 70 percent of the total decay heat generated during a period of 50 years after the first waste is emplaced (CRWMS M&O 2000 [DIRS 120903], Section 6.5). A conservative model, accounting only for heat removed as sensible heat in the ventilation air (ignoring latent heat removed by evaporation of moisture), indicates that a ventilation air flow rate of up to 15 m^3/s in each emplacement drift will provide this level of heat removal (CRWMS M&O 2000 [DIRS 120903], Section 6.5). The remaining heat output during the preclosure period will be transferred to the host rock by radiation, conduction, and convection, increasing the host rock temperature.

5.2.2 Information Generated by the Multiscale Thermal-Hydrologic Model

Results of the MSTH model are discussed below. Additional plots of results are available in the *Multiscale Thermohydrologic Model* report (CRWMS M&O 2000 [DIRS 149862]) and *Abstraction of NFE Drift Thermodynamic Environment and Percolation Flux* (CRWMS M&O 2001 [DIRS 154594]).

Figure 5.2-4 shows the computed average CSNF waste package temperature for the five infiltration bins (CRWMS M&O 2001 [DIRS 154594], Section 6.1) in the mean-infiltration case. The infiltration fluxes are discussed in Section 3.3.2. A large temperature increase occurs shortly after closure of the potential repository (50 years after emplacement) when ventilation ceases. During cool down, waste packages near the potential repository edge cool faster than waste packages in the center of the potential repository. The waste packages in the 0- to 3-mm/yr and the greater than 60-mm/yr infiltration bins cool faster than the others because all locations in those bins are at the edges of the potential repository (Figure 5.2-3). The differences among the infiltration bins are greatest during the early cooling period. By 10,000 years, the temperature of all the bins has converged and temperatures return to approximately ambient temperature. The results from the MSTH model for codisposal waste packages (codisposal waste packages have slightly lower temperatures because of a lower heat output) are quite similar to those for CSNF packages (CRWMS M&O 2001 [DIRS 154594], Section 6.3.2).

Figure 5.2-5 shows the computed average CSNF waste package relative humidities for the five infiltration bins in the medium-infiltration case. The relative humidity decreases sharply when the temperature rises after ventilation ceases. However, the calculated preclosure relative humidity is artificially high in Figure 5.2-5, because removal of moisture by ventilation is not included in the model. As with the temperature results, the differences among the infiltration bins are greatest during the early cooling period. By 10,000 years, the bin-averaged relative humidity values are above 90 percent and all are within about 2 percent of each other; by 100,000 years the bin-averaged relative humidity values are essentially back to ambient (nearly 100 percent relative humidity). Corresponding to their lower temperatures, the codisposal waste package relative humidity values are somewhat higher than the CSNF waste package relative humidity values (CRWMS M&O 2001 [DIRS 154594], Section 6.3.3).

Figure 5.2-6 shows the computed average percolation flux 5 m above the emplacement drifts for the five infiltration bins in the medium-infiltration case. As expected, the percolation flux is higher for the higher-infiltration bins. Infiltration response to the climate changes is clearly visible at 600 years and 2,000 years. All five curves have a large spike at about 70 years due to the drainage of thermally mobilized water. The increased percolation flux could lead to a pulse of seepage into the drifts at that time. For most bins, the percolation flux in the figure does not decrease below the initial percolation flux, indicating that the boiling front usually does not extend out 5 m above the drifts.

5.3 UNCERTAINTY ANALYSES

The analyses of the evolution of the TH conditions are based on the predictive modeling of the MSTH model with associated uncertainties. Accommodating uncertainties in the assessment of performance requires recognizing that uncertainties exist, and explicitly identifying those that may be important to performance. The DOE approach to dealing with uncertainties is described in the S&ER (DOE 2001 [DIRS 153849], Sections 4.1.1.2 and 4.4.1.2).

Three basic approaches are used to deal with uncertainties. The first is to identify the important parameters (DOE 2001 [DIRS 153849], Sections 4.2.2.3 and 4.2.3) and establish probability distributions for them. When probability distributions can be determined, the uncertainty can be quantified. Some distributions can be determined from collected data. These distributions are used to estimate the probability that a variable will assume different values over the spatial and temporal scales of an operating repository. The uncertainties that can be quantified are incorporated directly into performance assessment results.

The second approach to evaluate uncertainty is to develop alternative models for key processes. This approach seeks to reduce uncertainties that cannot be readily quantified (i.e., the possibility that the models used for compliance analyses do not include, or accurately simulate, processes that may be important to performance). The alternative model approach is most applicable to scenarios that have uncertainties associated with an approach, assumption, or conceptualization incorporated within a model that cannot be readily quantified.

A third approach to evaluating uncertainty is to establish bounding values of parameters or bounding approximations for processes or models. Establishing bounds that parameter values are unlikely to exceed, while not quantifying the uncertainty, places limits on the uncertainty. Likewise, limits are determined beyond which the results are insensitive to the further variation in the value. Sensitivity studies can assist in establishing these bounds by considering the range of parameter values that influence the results. Thus, establishing bounding values can provide an evaluation of uncertainty influences on results where actual quantification of the uncertainty is either unachievable or impractical.

The first method provides quantitative estimates of the effects of the uncertainty on potential repository performance. Using alternative models can also help quantify the uncertainty by comparing the results. However, unless all alternatives are exercised, the quantification of uncertainty is not complete. Therefore, where all possible alternatives cannot be defined, the quantification of uncertainty using the alternative model approach would not be as rigorous as the probability distribution method. In contrast, the third method, establishing bounds, does not provide absolute quantification of uncertainty, but it is useful when the effects are difficult to quantify or when specific conditions are expected to have minor effects on overall performance of the potential repository. Sensitivity studies give insight into the impacts of uncertainties, but they do not quantify the uncertainties directly.

Variability in parameters is sometimes classified as an uncertainty. However, variability, in and of itself, is not an uncertainty. If the variability in properties is well constrained and can be understood or characterized well enough (through existing data or observation) to be described deterministically, then it need not be considered uncertain and need not be described probabilistically. However, if the variability is not sufficiently constrained or well understood, then uncertainty is introduced and the approaches to evaluating that uncertainty, including quantification of it, must be applied. Although this difference seems subtle, the influence on uncertainty is quite different. In the case where the variability is well understood and accounted for, analyses can be deterministic without variability introducing uncertainty. Where this is not the case, which is the more common occurrence, the variability introduces uncertainty that must be addressed.

As discussed in the *Near-Field/Altered-Zone Models Report* (Hardin 1998 [DIRS 100123], Section 1.4.2), heterogeneity is an intrinsic characteristic of geologic media, and the effect of heterogeneity on flow and transport cannot be removed by gathering more data on formation properties. However, the accuracy with which the effect of heterogeneity on flow and transport can be calculated may be improved. Uncertainty arises from imperfect knowledge of the variables and mathematical relations among them. Uncertainty can be reduced with additional data or better methods of interpolating between measured data.

Because variability usually is not sufficiently constrained or understood to allow the deterministic approach, in this section variability will be discussed within the context of parameter uncertainty. However, the general approach is the same: to quantify the variability, to establish appropriate bounds on the parameter, or to consider impacts through sensitivity studies.

5.3.1 Multiscale Model of In-Drift Thermal-Hydrologic Conditions

5.3.1.1 Goal of the Model

The overall goal of the MSTH model is to provide analyses of the temperature, relative humidity, and liquid saturation in the drift and surrounding rock to the TSPA. The MSTH model also supports models of seepage, engineered barrier system degradation, radionuclide transport, and flow and transport, and provides inputs to other coupled process model analyses. The MSTH model evaluates the effects of heat on vapor and liquid flow and the distribution of liquid and temperature within and external to the emplacement drifts. The areas addressed by the MSTH model include: (1) temperature and relative humidity conditions at various locations within the drift, (2) gas and liquid flow rates through the rock and into the drifts, (3) the extent of the two-phase zone induced by boiling or evaporation, (4) temperature and saturation changes in the unsaturated zone, and (5) removal of moisture and reduction of waste package temperatures through ventilation. However, only the aspects that relate to in-drift conditions are discussed in this section. The in-rock conditions are necessary to calculate the in-drift conditions, but are not reported here.

An important part of the model goal is to develop a mechanistic understanding of the impact of uncertainty sufficient to build confidence that the modeled results are applicable and can be relied on in assessing the potential health and safety impacts to the public. This section discusses the analyses that have been performed to identify and analyze those uncertainties. The process for identification and evaluation of the uncertainties that were performed for the TSPA-SR design (CRWMS M&O 2000 [DIRS 153246]) is presented first, followed by a discussion of the approaches that were used to address uncertainties not quantified by the TSPA analyses.

5.3.1.2 Representation in Total System Performance Assessment-Site Recommendation

Uncertainties associated with the MSTH model were evaluated to quantify their magnitudes or identify them as unquantified. Approaches were then developed to determine the significance of the unquantified uncertainties.

There are four types of thermal-hydrologic uncertainties, based on the source of the uncertainty. The first is the uncertainty associated with the thermal-hydrologic models and their assumptions, abstractions, numerical simplifications, or representations. The second includes uncertainties introduced by physical processes. The third type includes uncertainties introduced through model sensitivities to input data such as thermal conductivity, invert thermal properties, and invert hydrologic properties. The last type includes uncertainties associated with sensitivity to removal of heat and moisture through ventilation. The key uncertainties (grouped according to whether they are model, process, or input uncertainties) are summarized in Table 5.3.1.2-1, which also provides pointers to discussions of further analyses.

5.3.1.2.1 Model Uncertainty

The TH coupling of heat and mass transfer can be treated in a number of ways. For heat transfer, conduction models are the most straightforward; however, these fail to incorporate the coupling of heat transfer with moisture that can be dominant within the engineered barrier system and near-field environment. The MSTH model combines conduction with the effects of latent heat and advective heat transfer. The merging of conduction and convective submodels can introduce uncertainty. However, the model has been used effectively to analyze field tests. As noted in the *Multiscale Thermohydrologic Model* (CRWMS M&O 2000 [DIRS 149862], Section 6.13.2), there is good agreement between the model and the measurements made in the Drift Scale Test. The Drift Scale Test was designed to test the coupled process models, including the MSTH model, and is being conducted underground in the environment appropriate for testing these models. Based on the agreement between test measurements and the model, it is not expected that there are large uncertainties related to how the submodels are integrated. The agreement between the simulated and measured temperatures in the region close to the heated drift indicates that the representation of thermal radiation inside the heated drift is adequately represented in the Drift Scale Test implementation of the MSTH model.

Three different approaches have been used by the Yucca Mountain Site Characterization Project (YMP) to model the physical processes involving flow: the equivalent continuum model, the discrete fracture model (DFM), and the DKM approaches. Because they represent alternative models, the results can be compared to help determine the extent of uncertainties within the models. All three approaches are discussed for completeness; however, the MSTH model relies on the DKM approach. A more complete comparison of these methods, and the results of analyses using these methods, can be found in the *Near-Field/Altered-Zone Models Report* (Hardin 1998 [DIRS 100123], Section 3.3.3).

The equivalent continuum model treats flow of water and vapor as if it were occurring in a single continuum with properties that are representative of or equivalent to those of the separate rock matrix and fracture continua. The challenge for this approach is to determine the appropriate properties that are either equivalent to the combination of the properties in the separate continua or that yield results equivalent to those from assessing each continuum individually. Furthermore, this method does not recognize the potential for fundamentally different flow phenomena between fractures and pores within the rock matrix; rather, it treats the TH conditions as if complete equilibrium existed between the hydrologic conditions in the matrix and fractures. Because the equivalent continuum model does not treat fractures as discrete features, TH effects are averaged over the entire spatial domain. In effect, the equivalent continuum model assumes instantaneous heat and mass transfer between the matrix and fracture continua. It does not adequately address transient effects, such as transient, episodic infiltration. The assumption of local equilibrium between fractures and matrix is appropriate if the liquid-phase flux in the fractures is sufficiently small (Buscheck and Nitao 1991 [DIRS 121169]; Nitao et al. 1993 [DIRS 147403]).

The DFM treats TH conditions in the fracture and matrix separately. In this method, the separate continua do not overlap each other. While this method may be physically more accurate, it requires a complete understanding of the fracture, the matrix continua, and their interactions. To apply this approach to repository- or mountain-scale problems would require extreme amounts of data and computational effort. Because of mathematical limitations on the numerical solution of the relevant equations, the DFM can be applied only for the simplest geometry of fracture networks. In addition, these fracture networks must have a high degree of spatial symmetry so the model domain can be spanned by a practical number of gridblocks.

The DKM treats the matrix and fractures as separate but overlapping continua. While it does not incorporate actual fracture spacing—the fractures are accounted for by permeability applied over the same intervals as the matrix blocks (i.e., overlapping continua)—the DKM does account for interaction between the TH conditions within the two continua. The DKM treats the matrix and the fractures as two distinct porous continua, with transfer terms to represent the mass and heat flux between them. The DKM does not assume capillary pressure equilibrium between fracture and matrix continua. Two sets of properties (one for fractures, one for matrix) are associated with each geometric gridblock.

The MSTH model relies on dual-permeability continuum models with an active fracture model (AFM) to account for interactions between fractures and matrix. Because these models do not directly analyze the actual flow and fracture systems, there is uncertainty in the model. However, comparisons of the models against field tests indicate that the models are appropriate and that large uncertainties are not expected. The agreement between the simulations and measurements in the Drift Scale Test indicates that the LDTH submodels in the MSTH model, together with the use of the drift-scale hydrologic property set, are validated for their intended use (CRWMS M&O 2000 [DIRS 149862], Section 6.13.2).

The major assumptions that apply to the TH models are: the dual-permeability flow model, the van Genuchten/Mualem saturation-desaturation relations, the matrix and fracture hydrologic properties determined by inverse modeling, the active-fracture coupling model between matrix and fracture continua, and the lack of incorporation of small-scale heterogeneity. These assumptions were addressed in a peer review, which found them to be able to represent a range of infiltration rates without producing unphysical hydrologic properties (CRWMS M&O 1999 [DIRS 148463], p. 47, paragraph 3). However, the peer review identified several concerns regarding the physical meaning or defensibility of these assumptions. It was determined that these uncertainties cannot be individually quantified; their resolution depends on field and laboratory tests or experiments to confirm the appropriateness of this group of assumptions.

The AFM reflects the observation that the contact area for interaction between water in fractures and the pores of the rock matrix is not the same as the fracture-surface contact area. Laboratory and field studies support the understanding that flow in fractures does not occupy the entire fracture-system volume. Most of the studies, including laboratory studies, were conducted under isothermal conditions, and many laboratory studies relied largely on artificial (machined) fractures (Nicholl et al. 1994 [DIRS 141580]; Liu et al. 1998 [DIRS 105729]). Currently, the AFM uses a fracture-interaction factor that varies as a function of saturation within the fracture. Although the active-fracture concept is intuitive, it is based on inverse modeling to match saturation data from field tests, not on a detailed physical basis from laboratory studies (CRWMS M&O 2000 [DIRS 141187], p. 47). This introduces model uncertainty.

Modeling of ventilation effects by reducing waste package heat output by 70 percent, without considering dryout of the near-field rock, does not consider the processes of moisture and heat removal associated with the drying processes. Thus, air ventilation will more effectively remove heat and moisture, until the rock is dried, than the models would indicate if these processes are not included. Thus, neglecting the effects of moisture removal provides an upper bound on temperatures and drift wall saturations, and thus on uncertainty of the effects of ventilation on those thermal-hydrologic properties until such time as the moisture is removed so that the rock has dried out. At that time, the thermal conductivity would be that of the dry rock and if the models used the wet rock thermal conductivity, they would underpredict the temperatures. However, the temperature peaks during early times when the ventilation would most likely still be removing moisture. Therefore, those later time temperatures should remain below the calculated peak temperatures and underpredicting later temperatures should not exceed the bounding temperatures calculated. The saturations will be less than calculated because of removal by moisture and therefore this thermal-hydrologic property will be conservatively bounded by the MSTH model calculations.

The MSTH model only calculates the ratio of water evaporation rate to water flow rate for a porous medium. The evaporation rate and flow rate at the top of the drip shield cannot be directly calculated by the model for an open drift. Thus, the liquid flow rate at the drip shield is taken from the seepage abstraction (CRWMS M&O 2000 [DIRS 153246], Section 3.2.4), and the evaporation rate provided is bounded by the amount of heat available to vaporize water on the upper portion of the drip shield. These bounding values estimate how much water could be evaporated by waste package heat output at any given time (CRWMS M&O 2001 [DIRS 154594], Section 6.3.10). Seepage estimates are conservatively bounded; therefore, the uncertainty introduced by the lack of direct calculation should also be bounded. The evaporation rate (more specifically, the amount of liquid water that potentially would not evaporate) may not be bounded as well, since this approach does not consider other processes that could impact evaporation rates. However, the approach provides an upper bound on evaporation if ventilation effects are ignored. It can be argued that liquid water on drip shields and waste packages is more adverse than humid air and, therefore, that the MSTH model approach bounds the issue of concern. However, the presence of deliquescent salts can result in water film on the waste packages. Therefore, an assessment needs to be made to determine whether it can justifiably be assumed that liquid water, not humid air, is more adverse, and that bounding the amount of water that can be evaporated is an acceptable approach.

Localized effects of seepage on TH response were not included in the TH models. If seepage was included, relative humidity would be higher and temperatures would be lower at locations where seepage occurs. However, as shown in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246], Section 4.1.2), there is no seepage at about 87 percent of the waste package locations evaluated in the TSPA model. For the small fraction of locations with seepage, the effect on relative humidity and temperature would be significant only during the first few hundred years.

The MSTH model provides an approximation of heat transfer for different time scales by coupling submodels that reflect the differing scales. The approach relies on estimates of equivalent AMLs in the calculations and the use of scanning curves. This introduces uncertainty with respect to whether the heat transfer assumptions and conceptualizations in the various submodels, and the combining of the submodel results, adequately reflect the physical reality. This uncertainty is not quantifiable and requires testing or comparison against other approaches.

Another uncertainty that may impact the results of TH modeling includes the arrangement and heat output of different types of waste packages. This engineering heterogeneity can influence the details of TH responses within the drifts. While the uncertainties are a function of the final design and cannot be entirely assessed at this time, agreement with field test data indicates that the model approaches are appropriate for determining this influence (CRWMS M&O 2001 [DIRS 149862], Section 6.13.2).

The stochastic representation of fracture heterogeneity in the seepage model is not incorporated in the MSTH model. Conversely, the seepage model for the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) did not include dryout and heating of the near-field rocks to couple these models. The MSTH model was used to predict percolation flux in the host rock 5 m above the drift wall, which was then used as input to the seepage model for calculating seepage during the thermal pulse. This introduces an uncertainty about the applicability of the model. However, the impacts of seepage are bounded because the thermal percolation flux at 5 m is modeled as flowing into ambient temperature and saturation rock. This is a conservative approach that ignores the temperature and seepage mitigation processes of evaporation and imbibition in the near-field rock during the thermal period. The effects of seepage during the thermal period on the temperature and relative humidity in the emplacement drifts were evaluated independently using the MSTH model, to determine the influence of seepage on in-drift thermal-hydrologic conditions. These effects were found to be negligible for the relatively small but bounding values of seepage that could occur (CRWMS M&O 2000 [DIRS 149862], Sections 6.11 and 6.12).

The multiscale estimation methodology does not include the effects of mountain-scale gas-phase convective circulation (at a scale larger than the lateral size of the LDTH columns, approximately 40 m) and the movement of water vapor along the axis of emplacement drifts from warmer to cooler regions. The multiscale modeling approach neglects heat transfer by these mechanisms, so the predicted temperatures and the duration of the thermal period are probably overpredicted. The principal effect on TSPA is probably a delay in calculated time of the return of moisture to the in-drift environment. However, differences in timing on the order of hundreds of years will have a minor impact on the estimated longevity for the drip shield and waste package (with expected lifetimes greater than 10,000 years).

5.3.1.2.2 Uncertainties in Physical Processes

There are potential changes to hydrologic properties in the surrounding rock caused by coupled thermal-hydrologic-chemical (THC) and thermal-hydrologic-mechanical (THM) processes. Based on prior evaluations of their significance, such changes were not addressed (CRWMS M&O 2000 [DIRS 153246], Section 3.3.3.1.2). Previous analyses (BSC 2001 [DIRS 154677]) concluded that chemical processes would not cause significant changes to hydrologic properties. These analyses considered the mass balance of mineral dissolution and deposition within the fractures. They also considered dissolution and deposition to be uniform within the entire fracture porosity represented in grid elements no smaller than a few tens of centimeters. There remains an unquantified uncertainty related to whether the uncertainty in fracture porosity, the heterogeneity in fracture porosity, or the localized deposition of minerals that could cause smaller than gridblock-sized plugging of fractures could change this conclusion. The report *Calculation of Permeability Change Due to Coupled Thermal-Hydrological-Mechanical Effects* (CRWMS M&O 2000 [DIRS 149040]) also concluded that fracture permeability could increase by an order of magnitude due to irreversible shear movement. However, this increase was determined to be within the range of fracture permeability variability. Therefore, the influence of THC and THM coupling was not incorporated into the MSTH model. The uncertainty to be evaluated is whether heterogeneity of fracture porosity, localized deposition, or design changes (such as orientation of drifts relative to the fracture patterns) could change the previous conclusions.

Boiling point temperatures are a function of pressure imposed on a liquid. The physics of this process is well understood and has been incorporated into the MSTH model. The MSTH model is comprised of four submodels that are discussed in Section 5.2. However, the models must calculate the increase in pressure based on the permeability of the rock matrix and the size of the matrix blocks. Fracture permeability is sufficiently high that pressures will not build up within the fractures, so this phenomenon is not applicable to the fracture continua. Therefore, although the process is understood, there is uncertainty regarding the characterization of the matrix block. These uncertainties are the same as those for unsaturated zone flow, and are discussed in Section 3.3. No assessment is made in the TH models of changes in capillary pressure based on potential changes in fracture porosity due to coupled processes. It is judged that this is of lesser importance than other processes. Small changes in capillary pressure would not have a significant impact because of the existing wide distribution of pore sizes, and thus capillary pressure, in the rock. Therefore, the uncertainties from this factor are expected to fall within the existing variability in capillary pressure and would not be significant.

However, testing wafers of welded tuff have indicated that the heating history may have some effect on moisture retention in the rock. Tests show that the suction potential decreases much more rapidly with increasing saturation during wetting than it does during drying (Wilder 1996 [DIRS 100792], Section 2.1.1). This hysteresis, where more moisture is retained in the samples during drying than during subsequent wetting, is not as pronounced at elevated temperatures, and at 93.6°C, the hysteresis was reversed. No process has been identified that can explain smaller hysteresis at 78°C than at other temperatures, or explain the hysteresis reversal at 94°C; in this test, the samples were heated from 25°C to 94°C, then cooled to 78°C. Thus, the heating history may have some effect on the moisture retention curves. Rewetting behavior at an elevated temperature was also summarized in the *Syntheses Report on Thermally Driven Coupled*

Processes (Hardin and Chesnut 1997 [DIRS 150043], Section 2.7.5), which reports similar decreases in hysteresis with temperature but not the reversal in hysteresis. The hysteresis effect is probably related to changes in surface tension and the rock-water-air contact angle at elevated temperatures (Hardin and Chesnut 1997 [DIRS 150043], Section 2.10). Hysteritic behavior is generally ignored, for computational expediency, in TH models. It has been judged that this appears to be defensible (DOE 2001 [DIRS 153849], Section 4.2.2.2.2). The effects would be to overpredict imbibition or rewetting. Therefore, ignoring this hysteresis would result in conservatively (upper) bounded values of rewetting. However, ignoring this factor may not result in conservative bounds on peak drift wall temperatures. If the dryout of rock is underpredicted (i.e., wetting is overpredicted), the result may be the use of wet rather than dry thermal conductivities in the model. Thermal conductivities for wet rock are higher than for dry rock, so the calculated temperatures would be lower.

5.3.1.2.3 Input Data Uncertainties

The unsaturated zone flow model (CRWMS M&O 2000 [DIRS 151940]) is the basis for the hydrologic properties used as inputs to the MSTH model. There are uncertainties associated with the use of inverse modeling to determine the physical properties that are used in the MSTH model. Therefore, uncertainties associated with the unsaturated zone flow model, such as uncertainties in the average infiltration rate as a function of climate (CRWMS M&O 2000 [DIRS 153246]), also apply to the MSTH model. The assessment of uncertainties in these properties is discussed within the context of the unsaturated zone (mountain-scale) model (Section 3.3.5) where property distributions are determined. However, the impact of propagating these uncertainties through the TH models has not been directly quantified. Sensitivity studies performed with the MSTH model have been compared to field tests and the appropriate property set determined (BSC 2001 [DIRS 154677]). As noted previously, there was good agreement between the MSTH model simulations of the Drift Scale Test and the measured parameters (CRWMS M&O 2000 [DIRS 149862]). This agreement indicates that the drift-scale hydrologic property set used as input to the modeled simulations is valid for its intended use.

The effects of percolation flux variability, beyond those accounted for in the detailed chimney models, have not been included (CRWMS M&O 2000 [DIRS 149862], Section 1.0 and Figure 1-1). Variability is described by a distribution of infiltration. Three infiltration cases (low, medium, and high) are considered in the MSTH model. The infiltration values included in the chimney models incorporate the distribution of measured values that reflect the impacts of topography, ground cover, and stratigraphy on the distributions. Because the distributions are quantified, this uncertainty is considered to be quantified. In addition to incorporating uncertainties in percolation flux by considering the low, mean, and high infiltration flux conditions, the MSTH model considers temporal variability (e.g., changes in climate) and spatial variability (e.g., repository cooling at the edges) in the models. To this extent, this is a quantified uncertainty.

The waste package thermal output depends on design and operating details that are not finalized. Thus, the output used in the MSTH model may not accurately reflect the output of actual waste as it would be emplaced. Likewise, the final potential repository layout, ventilation, and waste package arrangement may be different than the one analyzed in the current MSTH model calculations. This uncertainty does not add to the uncertainty of the analyzed conditions, which use specific design parameters. What this uncertainty underscores is the ultimate need to perform MSTH model calculations for the final design and repository conditions that will be considered during any potential license application and decision to emplace waste.

Uncertainty is also introduced into the MSTH model from the uncertainties associated with lithophysal porosity (see Section 3.3.5). The uncertainty introduced into the MSTH model almost entirely relates to the impact on thermal conductivity and heat capacity used in the models for the lower lithophysal unit. Higher porosity results in lower the thermal conductivity and heat capacity of the rock. Thus, if the porosity is higher than the value used to determine these parameters, the transient temperature rise may actually be greater than that calculated by the models. This uncertainty would be of diminishing concern with time, although, as discussed in Section 5.3.1.4.8, effects of thermal conductivity can persist for 10,000 years for the HTOM. The effects of heat capacity uncertainty, as noted in Section 5.3.1.4.9, disappear within 1,000 years after emplacement. For the LTOM, the magnitude and duration of effects would be less than those indicated.

Lithophysal porosity can also affect the effective porosity for vapor storage. If the porosity is considerably larger than that used in the models, then there may be a lag in how quickly water vapor moves through the system compared to the models. During active boiling periods, this would create uncertainty in the temperatures that develop and in the amount of water mobilized. If the vapor is stored so that it does not move as rapidly or as far, then moisture will remain closer to the drifts and temperatures will not be as high. Therefore, this uncertainty would tend to result in conservative estimates of temperature, but possibly nonconservative estimates of saturation and moisture conditions in the rock adjacent to the drifts. Whether this uncertainty persists beyond the active boiling period will depend on how effectively the rock stores the water, thus adding to uncertainty. However, as noted in Section 5.3.1.4.1, the magnitude of this uncertainty is not expected to be large. Vapor storage would be less of an issue, if at all, for LTOM where temperatures in the rock would be below boiling.

Uncertainty in thermal conductivity is mainly related to the difference between wet and dry rock thermal conductivity. While thermal conductivity is a function of the porosity and mineralogy of the rock, there is not much variability in thermal conductivity as a result of these factors, and the values can be bounded. However, there is a significant difference between the thermal conductivities of wet and dry rock. Because the moisture conditions can vary both spatially and temporally, and because the moisture conditions are calculated by the TH models, this uncertainty is not as easily bounded. Thermal conductivity always influences the temperatures calculated. Because some processes are not incorporated into the models (e.g., rewetting hysteresis), it is possible that wet thermal conductivity will be used when a dry thermal conductivity would be more appropriate. This would result in underprediction of temperatures but overprediction of moisture conditions.

Finally, there is uncertainty in the value of heat capacity used in the models. As noted, porosity can influence the heat capacity. However, because heat capacity is only important to temperature calculations during the thermal transient phase (as noted in Section 5.3.1.4.9, the effects disappear within 1,000 years of emplacement), and because it becomes unimportant after that period, the uncertainty introduced is not judged to be significant.

5.3.1.3 Reduction in Total System Performance Assessment Uncertainty Due to Model Improvements

In Section 5.3.1.2, uncertainty was grouped into three major categories: model uncertainty, process uncertainty, and input data or parameter uncertainty. This section discusses work performed after the issuance of the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) that reduces the uncertainties discussed in Section 5.3.1.2. Improvements in the models used in the Volume 2 (McNeish 2001 [DIRS 155023]) TSPA include consideration of two of the three design cases outlined in Section 5.1: the above-boiling case and the low temperature (85°C) on the surface of the waste package case. The third design case, limiting drift wall temperatures to sub-boiling, was not considered in the SSPA (Table 5.1-1). These model improvements allow for identification of parameters and conditions that are sensitive to design details, thus helping to reduce the uncertainties related to use of a single design case for analyses. In addition, after the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) analyses, sensitivity studies and other analyses were performed to consider the consequences of additional uncertainties.

Improvements were made to the multiscale TH models (MSTH model) (CRWMS M&O 2000 [DIRS 149862]) in the way the submodels are constructed and combined. The improved smeared-heat-source mountain-scale thermal (SMT) submodel includes a depiction of the Yucca Mountain potential repository layout that more accurately represents the locations of the potential repository edges and the emplacement drifts. The version of the MSTH model used in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) accurately reflected the eastern repository boundary and depicted the western boundary with some approximations. The northern and southern boundaries, however, were not as well represented. Figures 5.4.1-1 and 5.4.2-1 show the SSPA model depictions of the potential repository layout.

The drift-scale submodels in the MSTH model used in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) used a square representation of the drifts. The improved submodels incorporate a stair-step grid approximation of the circular emplacement drifts (Figure 5.3.2.3-1). Although an analysis (CRWMS M&O 2000 [DIRS 149862], Section 6.5.2) in support of the TSPA-SR determined that the impacts of the square approximation were not significant, the use of a near-circular shape reduces the associated uncertainty.

The DDT submodel has also been modified since the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) to directly incorporate thermal radiation connections both inside and outside the drip shield. This is a more rigorous approach that allows for direct calculation of radiative heat transfer. It removes the uncertainties associated with using different approaches and approximations for temperatures at locations below the drip shield (where radiation connections were used) and outside the drip shield (where effective thermal conduction approximations based on changing temperatures were used). This improved approach addresses some of the uncertainty identified in Table 5.3.1.2-1 as "coupling of submodels." As discussed in Section 5.3.2.4.5.2, using correlation-based effective thermal conductivity parameter for thermal radiation under predicts the early time temperatures at the drip shield (compared to using explicit thermal conductivity from radiation). As described in Section 5.3.1.4.2, from closure of the potential repository until about 1,000 years, the effective parameter for thermal radiation underpredicts the average surface temperature of the drip shield by as much as 10°C at closure of the potential repository. The peak temperature on the drip shield is underpredicted by the effective parameter by about 5°C at closure of the potential repository. At 1,000 years, the temperature defect is about 1°C.

The effective thermal conductivity used in the MSTH model for natural convection was revised (see Section 5.3.2.4.5) based on repository-wide average temperatures instead of a selected subset at the potential repository center, as was used in the MSTH AMR (CRWMS M&O 2000 [DIRS 149862], Section 5.3 in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]). An explicit representation of thermal radiation heat transfer from the heat source to the drift wall was used to generate the temperature time-histories applied to the development of a new time-dependent effective thermal conductivity for natural convection. The effective thermal conductivity governs the approximate rate at which heat is transferred from the heat source to the drift wall. By its very nature, the effective thermal conductivity is temperature-dependent. Therefore, a more representative temperature will decrease the uncertainties in the rate of heat transfer and, thus, in the calculated temperatures.

The setup of the spatial grids (for solution of the finite difference approximations to the differential equations) in the DDT submodel for the areas outside the drip shield has been made identical with the grids used in the LDTH submodel. This helps to address the model uncertainty identified in Table 5.3.1.2-1 as "coupling of submodels," and removes problems that could be created by mismatches in information passed across gridblocks.

The improved MSTH model more accurately reflects edge effects. Previously, the submodels used a fixed, effective, local areal mass loading (AML), selected based on the peak temperature for that location. The improved approach continues to use the nominal AML initially, but uses an evolution of the local effective AML to reflect the time-varying influence of edge cooling. This capability is incorporated into the LDTH and DDT submodels; therefore, all thermal interactions that reflect the evolving influence of edge effects are addressed in the improved models. The edge effects are illustrated in Figures 5.4.1-4 and 5.4.2-4, which show snapshots in time of the distribution of temperature across the potential repository footprint for the HTOM and LTOM, respectively.

The improved MSTH model also accounts for the presence of lithophysae, which can cause uncertainties in the models from multiple standpoints. First, uncertainty is generated from the effects of lithophysal porosity on the storage capacity of the rocks for vapor (the conceptualization is that the cavities will not fill with water), as discussed in Sections 4.3.5.3.2 and 5.3.1.4.1. Second, lithophysal porosity can influence thermal conductivity, as discussed in Sections 4.3.5.3.2 and 5.3.1.4.9. The TSPA-SR analyses (CRWMS M&O 2000 [DIRS 153246]) used thermal conductivity based on water-filled lithophysae.

The way that steel in the invert is incorporated into the models has also been improved since the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]). Previous models based thermal conductivity measurements for the steel in the invert on intact, non-degraded steel. However, for most of the time of concern, the steel will have been significantly degraded by corrosion, so thermal conduction will not be as high as assumed. In the updated models, the thermal conductivity used for the steel components was the same as that of the crushed tuff. This value was selected based on an assessment that the steel would completely degrade and that the iron rust would have thermal conductivity similar to that of the rock. This will result in higher in-drift temperatures, and thus will be more conservative relative to the peak temperatures within the drift. This approach addresses, partially, the uncertainties identified in Table 5.3.1.2-1 as "Invert Properties-Input Data Uncertainty."

5.3.1.4 Quantification of Uncertainty Using Process Models

In addition to reducing model uncertainties by incorporating improvements to the multiscale thermal hydrologic model (MSTH model), sensitivity analyses were performed to further evaluate the consequences (or quantification) of uncertainties in processes and model inputs. Before and after the TSPA-SR analyses were conducted (CRWMS M&O 2000 [DIRS 153246]), sensitivity studies or other analyses were performed to consider the consequences of the uncertainties in eleven areas. These analyses were conducted to improve confidence in the models supporting the TSPA, but they do not provide inputs directly to the Volume 2 SSPA (McNeish 2001 [DIRS 155023]). The results of these analyses are discussed in the subsequent Sections of 5.3.1.4. These sections address uncertainty elements introduced in Section 5.3.1.2 and Table 5.3.1.2-1.

The areas in which uncertainty consequences were analyzed are:

1. Sensitivity of TH results to neglecting the potential for vapor storage within the lithophysal cavities (porosity). Current models do not provide analyses of cavity storage separate from the overall fracture porosity in the DKM model (Section 5.3.1.4.1)

2. Sensitivity of in-drift temperature and relative humidity to the effects of heterogeneous fracture properties on seepage. Previous models did not incorporate the effects of heterogeneity on seepage or on MSTH model results. Seepage was determined based on average or representative fracture properties, considering both variability and anisotropy (Section 5.3.1.4.2)

3. The impacts of imbibition hysteresis noted for intact samples under wetting and drying conditions (Section 5.3.1.4.3)

4. Sensitivity studies of the impact of mountain-scale buoyant gas-phase convection on temperatures and their durations (Section 5.3.1.4.4)

5. Effects of THC coupled processes, especially those related to changes in hydrologic properties (Section 5.3.1.4.5)

6. Effects of THM coupled processes related to changes in hydrologic properties (Section 5.3.1.4.6)

7. Sensitivity of MSTH model results to uncertainties in the bulk permeability of the host rock. Bulk permeability is used as an input to the multiscale TH models, so uncertainty in this parameter might cause uncertainty in the results (Section 5.3.1.4.7)

8. Sensitivity of MSTH model results to uncertainties in the host rock thermal conductivities used in the models (Section 5.3.1.4.8)

9. Sensitivity of the TH models to the way lithophysal porosity impacts other input parameters, such as bulk or host rock thermal conductivity (Section 5.3.1.4.9)

10. Sensitivity of the TH models to uncertainties in the thermal conductivity of the invert materials and in how they are incorporated into the models (Section 5.3.1.4.10)

11. Sensitivity of the TH parameters to design and operational parameters (Section 5.3.1.4.11).

5.3.1.4.1 Effects of Lithophysal Porosity on Vapor Storage

The MSTH model and other hydrologic models use the DKM, in which the matrix and fracture continua consider two-phase flow (vapor and liquid). Previous analyses combined lithophysal porosity with fracture porosity, and assumed the combined porosity could be saturated under some circumstances. Although unanticipated processes (i.e., those that allow for localized saturation) could allow water to fill the lithophysal cavities, it is unlikely that this would occur in a freely draining unsaturated zone. Further, it is recognized that the physical processes that determine if seepage will occur into openings (drifts) also apply to the lithophysal cavities. Thus, it is likely that the lithophysal cavities will be unoccupied by water, except for film on cavity walls, and therefore will be entirely gas or vapor filled. This is consistent with observations that secondary mineral deposits are limited to the bottom of cavities and footwalls of fractures, and that they were deposited in unsaturated conditions (Whelan et al. 2001 [DIRS 154773], p. 6).

Gas-filled lithophysal cavities would provide a storage volume for water vapor from the boiling zone. Discussion of the uncertainty due to not separately incorporating this porosity into the thermal-hydrologic models is discussed in Section 4.3.5.3.2. The most important influence of lithophysal porosity will be on thermal conduction due to lower conductivity for air-filled voids than for rock matrix. The analyses of the effects of lithophysal porosity on thermal conductivity, and in turn, on in-drift temperatures, are discussed in Sections 5.3.1.4.8 and 5.3.1.4.9.

Neglecting vapor storage within lithophysal porosity is not expected to have a significant effect on the MSTH model results because of the magnitude of expansion of water as it goes from liquid to vapor phase. One pore-volume of water will result in 1000 pore-volumes of vapor (Ellenwood and Mackey 1962 [DIRS 154867], Plate 4C). The matrix and lithophysal pore volumes are similar, so the combined porosity is roughly double the pore-volume of the liquid that would be vaporized. Therefore, the error introduced by neglecting the vapor storage capacity of lithophysal porosity within the computational elements is the difference of accounting for one- instead of two pore-volumes of vapor (out of the 1,000 pore-volumes of vapor generated) that are not displaced to the next computational element. This results in a 0.1 percent overcalculation of the amount of vapor displaced to the next zone in the numerical model.

The uncertainty introduced by neglecting this 0.1 percent of the vapor displaced is less than would result from not accounting for the porosity heterogeneity among zones of the numerical model. The range of porosity for the potential repository units is from 10 to 60 percent (Mongano et al. 1999 [DIRS 149850], p. 17), a six-fold range of porosity. Thus, porosity averaged over zones in the numerical model would have a greater impact on storage than would neglecting lithophysal porosity (one-fold versus six-fold effects).

5.3.1.4.2 Effects on In-Drift Temperature and Humidity of Fracture Heterogeneity Aspects of Seepage

Uncertainties in MSTH model results can be introduced by heterogeneous seepage resulting from fracture property heterogeneity. These uncertainties are listed as model uncertainty in Table 5.3.1.2-1, Items 6 and 7. Analyses of the influence of seepage heterogeneity were conducted, subsequent to the MSTH model analysis (CRWMS M&O 2000 [DIRS 149862]), to address the in-drift environment uncertainties associated with the limited evaluations of seepage in the MSTH model. The two-dimensional LDTH submodel was used in the original MSTH model analysis. Because the MSTH model incorporates LDTH submodels at 31 locations in the potential repository, it captures the influence of repository-scale variability of hydrologic properties and conditions (e.g., infiltration flux). However, as incorporated in the original MSTH model analysis, the two-dimensional LDTH submodels did not account for the influence of drift-scale heterogeneity such as the influence of drift-scale heterogeneity of fracture properties, including permeability, porosity, and the capillary properties (the most important being the van Genuchten α parameter).

Over nearly the entire range of infiltration-flux conditions considered in the MSTH model (CRWMS M&O 2000 [DIRS 149862]), seepage into the drift is not predicted to occur. Nonzero drift-seepage fluxes were only predicted to occur in regions of the potential repository having the highest infiltration (and percolation) flux for the "upper" infiltration-flux case. An important reason for the low occurrence of predicted drift seepage is the assumption (in the LDTH submodel) of a uniform fracture continuum within any given hydrostratigraphic unit (particularly the host-rock units). This is equivalent to assuming no drift-scale heterogeneity of fracture properties in the host rock. This assumption, together with the use of a two-dimensional LDTH model, reduces the tendency for the occurrence of drift seepage to be predicted.

Previous studies of both isothermal and nonisothermal seepage (Tsang et al. 1997 [DIRS 123761]; Nitao 1997 [DIRS 100640]; Hardin 1998 [DIRS 100123], Section 3.6) indicate that with heterogeneous fracture properties, average seepage rates increase and the threshold for seepage decreases. Therefore, a sensitivity study with a three-dimensional LDTH model using heterogeneous fracture properties was conducted to determine what thermal-hydrologic variables predicted by the MSTH model would change as a result of drift-scale fracture heterogeneity.

The sensitivity analyses of the effects of heterogeneous fracture properties on in-drift conditions were conducted by selecting eight sets of fracture properties, from the stochastic realizations of fracture properties (Table 5.3.1.4.2-1). These sets were chosen not to be representative, but rather to assure that seepage could occur under all of the climate infiltration-flux conditions considered for Yucca Mountain. The selection of these sets should not be interpreted as being an indication of whether such heterogeneous conditions are realistic. Rather, they should be regarded as extreme examples of fracture heterogeneity that were selected to substantially challenge the hypothesis that boiling conditions at the drift wall are capable of thwarting seepage. They will, thus, result in conservatively bounded analyses. Therefore, the objective of these analyses, which used the *Three-Dimensional Heterogeneous LDTH Model from the MSTH,* REV 00/ICN 02A, model (BSC 2001 [DIRS 155007], Section 6.14), were to determine: whether fracture heterogeneity can result in liquid-phase flow penetrating through the boiling zone and result in a reduction in the duration of boiling, and to determine which in-drift thermal-hydrologic variables predicted by the MSTH model would be most significantly influenced by drift-scale fracture heterogeneity. In these sensitivity studies, the drift wall was an interface between materials (rock and porous-medium-air) that have different permeability. This approach allowed water to directly seep into the drift in the calculation.

The three-dimensional heterogeneous LDTH submodels used were based on the two-dimensional LDTH submodel at the L4C3 location (CRWMS M&O 2000 [DIRS 149862]), which is close to the geographic center of the potential repository. The host rock unit at this location is the tsw35 model unit (Tptpll unit), which is the predominant host rock unit in the potential repository. The mean infiltration-flux case was used. The L4C3 location has infiltration fluxes that are higher than the potential repository averages (BSC 2001 [DIRS 155007], Table 6-7).

The lateral gridding in the two-dimensional and three-dimensional LDTH models was slightly more refined outside the drift than was used in the original calculations (CRWMS M&O 2000 [DIRS 149862]. The finer gridding was used to assure that drift-scale heterogeneity would be represented with adequate resolution in the immediate vicinity of the drift. The three-dimensional LDTH model has an axial dimension of 5 m (approximately the length of one waste package), and it treats the upper 39.7 m of the host-rock unit (Tptpll) (17.4 m above and 16.8 m below the drift) from the drift to the mid-pillar location as having heterogeneous fracture properties.

As was noted, eight stochastic realizations were modeled (Table 5.3.1.4.2-1). All stochastic realizations used a log-normal distribution with values of $\log_{10}$ standard deviation and correlation lengths in the principal directions. In the heterogeneous fracture field, fracture permeability was assumed to be isotropic (as it is assumed in the hydrostratigraphic units that have homogeneous fracture permeability). Four of the realizations were for an AML of 56 MTU/acre, which is representative of heating conditions at the center of the potential repository. Four of the realizations were for an AML of 34 MTU/acre, which is representative of heating conditions close to the potential repository edge. The stochastic realizations were chosen in pairs (one for center and one for edge) to:

- Consider cases with greater potential for flow focusing, and thus seepage, by including greater heterogeneity than was noted in the field (Table 5.3.1.4.2-1, Cases A and B) and greater vertical correlation. These cases have a $\log_{10}$ standard deviation of 1.5, which is greater than the value of 0.72 determined from air-permeability data performed at Niche 3650 (CRWMS M&O 2000 [DIRS 153045], Table 4, p. 38) and also include a factor of 8 greater correlation length in the vertical direction.

- Evaluate the effects of excluding the relation between permeability and capillary strength (lower capillary strength associated with higher permeability) by assuming a constant value of capillary strength. Cases A and B (Table 5.3.1.4.2-1) were the same except that Case B used a constant value of capillary strength, whereas Case A used the capillary-strength parameter ($1/\alpha$) correlated to the heterogeneous fracture permeability field according to Leverett's scaling rule (Leverett 1941 [DIRS 100588], p. 159).

- Consider effects on seepage of slightly greater heterogeneity than measured in Niche 3650 (log_{10} standard deviation of 1 compared to 0.72), but without vertical biasing (Table 5.3.1.4.2-1, Case C), and to consider the effects of greater heterogeneity with a log_{10} standard deviation of 2.3 (Table 5.3.1.4.2-1, Case D) but with less focusing than Cases A and B (2x compared to 8x vertical correlation). More detailed discussion of these cases and their objectives is contained in the draft update to the MSTH model AMR (BSC 2001 [DIRS 155007], Section 6.14.4).

Detailed results follow:

- Seepage can vary from none to nearly the full amount of the percolation flux for fracture heterogeneity, as the permeability varies from slightly above that measured in underground tests (Case C) to very heterogeneous fracture properties. Table 5.3.1.4.2-2 summarizes seepage conditions in the drift after TH conditions return to near-ambient.

- The likelihood and magnitude of seepage increase with the log_{10} of the standard deviation of the fracture permeability (BSC 2001 [DIRS 155007], Section 6.14.5).

- The likelihood and magnitude of seepage increase with the ratio of vertical to horizontal correlation length. (BSC 2001 [DIRS 155007], Section 6.14.5).

- Correlating the capillary-strength parameter [$1/\alpha$] of the fractures with the fracture permeability according to Leverett's scaling rule resulted in a greater seepage magnitude than cases for which [$1/\alpha$] was constant (BSC 2001 [DIRS 155007], Section 6.14.5).

- The duration of boiling is never reduced as a result of fracture heterogeneity (BSC 2001 [DIRS 155007], Figures 6-83a, 6-83c, and 6-84), and the duration of boiling is slightly greater for the heterogeneous cases than for the homogeneous cases. The greater duration of boiling for the heterogeneous cases results from the influence of buoyant gas-phase convection being reduced by the heterogeneous fracture-permeability distribution (low-*k* features obstruct buoyant gas-phase convection). Thus, buoyant gas-phase convection plays a less significant role in the rate of cool down in the drift for the heterogeneous cases than for a corresponding homogeneous.

- Temperatures at the drift wall or on the drip shield are insensitive to heterogeneity during the boiling and post-boiling periods, with the exception that there is a slight increase in the duration of the boiling period for the heterogeneous cases (BSC 2001 [DIRS 155007], Section 6.14.5).

- Relative humidity in the drift is unaffected by fracture heterogeneity during the boiling period (BSC 2001 [DIRS 155007], Figures 6-83b and 6-83d).

- Relative humidity reduction in the drift is diminished during the post-period only for cases where seepage contacts the drip shield (BSC 2001 [DIRS 155007], Figures 6-83b and 6-83d). This effect decreases with decreasing seepage flux onto the drip shield (BSC 2001 [DIRS 155007], Figures 6-93d and 6-94d). For cases with no seepage flux onto the drip shield, the relative humidity reduction is not diminished (BSC 2001 [DIRS 155007], Figures 6-95d and 6-97d).

- For heterogeneous cases with seepage flux contacting the drip shield, the evaporation rate on the drip shield is greater than the evaporation rate for the corresponding homogeneous case (BSC 2001 [DIRS 155007], Figure 6-85) or for the heterogeneous cases with no seepage contacting the drip shield. This observation only applies to the post-boiling period because there is no seepage during the boiling period for the heterogeneous cases or the corresponding homogeneous cases; consequently, there is virtually no evaporation on the drip shield for the heterogeneous or homogeneous cases during the boiling period.

Summary–The results of the seepage analyses indicate that no seepage will occur during the boiling period, regardless of the fracture property heterogeneity. This study indicated that the in-drift thermal-hydrologic conditions calculated (CRWMS M&O 2000 [DIRS 149862]) would not be changed during the boiling period by virtue of adding the influence of drift-scale fracture heterogeneity. Further, the study found that the duration of boiling was not reduced as a result of fracture heterogeneity. These results, which are consistent with those using a different model in Chapter 4, justify the neglect of seepage in calculating the in-drift TH conditions.

For the post-boiling period, heterogeneity influences the seepage potential (BSC 2001 [DIRS 155007], Section 6.14.5), and can do so significantly, with seepage varying from 0 to as much as 86 percent of percolation flux for heterogeneous fracture systems with strong vertical correlation. The likelihood and magnitude of seepage increase with the $\log_{10}$ of the standard deviation of the fracture permeability, and further with the ratio of vertical to horizontal correlation length.

Temperatures were insensitive to heterogeneity during both the boiling and post-boiling periods, with the exception that there is a slight increase in the duration of the boiling period for the heterogeneous cases. In-drift relative humidity was unaffected by fracture heterogeneity during the boiling period, and diminished during the post-boiling period only for cases where seepage contacts the drip shield. For cases with no seepage flux onto the drip shield, relative humidity reduction was unaffected by heterogeneity.

If seepage flux contacts the drip shield, the evaporation rate on the drip shield will be greater for heterogeneous cases than the corresponding homogeneous case or the heterogeneous cases with no seepage contacting the drip shield.

5.3.1.4.3 Effects of Imbibition Hysteresis

The primary issue for capillary (or imbibition) hysteresis concerns matrix flow. The capillary properties of the matrix (quantified by the van Genuchten α and m parameters) are developed for drainage (or drying) conditions. Laboratory samples of the rock matrix are fully wetted and placed in a centrifuge, wherein water is incrementally removed by applying increasing suction potential. A moisture retention curve is developed, which is capillary pressure as a function of liquid saturation. Moisture retention data collected in this fashion is representative of the drying phase of the potential repository host-rock evolution. However, in all thermal-hydrologic modeling studies of the potential Yucca Mountain repository, these data are also assumed to be applicable to the rewetting of the host rock by capillary imbibition in the matrix. This assumption is equivalent to neglecting hysteresis between drying and imbibition behavior.

Imbibition hysteresis was discussed in Niemi and Bodvarsson (1988 [DIRS 155057]). The issue of imbibition diffusivity was addressed in the *Near-Field/Altered-Zone Models Report* (Hardin 1998 [DIRS 100123]). That report used the concept of the matrix imbibition diffusivity, which is a function of the van Genuchten α and m parameters, to compare the magnitude of matrix imbibition arising from various hydrologic property sets that had been used in thermal-hydrologic modeling studies of the potential Yucca Mountain repository. That report also determined the value of matrix imbibition diffusivity from the laboratory measurements of matrix imbibition of Flint et al. (1996 [DIRS 100676]). For all of the hydrologic property sets considered in Hardin (1998 [DIRS 100123] the values of matrix imbibition diffusivity were greater than that obtained from the laboratory measurements of matrix imbibition for the corresponding host rock unit. The differences in matrix imbibition diffusivity between the laboratory measurements and those determined from the property sets in Hardin (1998 [DIRS 100123], Table 3-3) probably are the result of capillary hysteresis; in other words, the imbibition diffusivity is less than the diffusivity for drainage conditions. For most of the potential repository host-rock units, the matrix properties for the base-case hydrologic property sets used in all TH calculations of the SSPA are similar to those of the 1997 TSPA-VA base-case hydrologic property set. Therefore, it is possible that the rate at which the dryout zone around emplacement drifts is rewetted by matrix imbibition is overpredicted by the TH model calculations in this report, including the MSTH model calculations.

Jury et al. (1991 [DIRS 102010], pp. 65 to 68) discuss the hysteresis in moisture content in the relationship of moisture potential versus volumetric moisture content. Moisture potential is not uniquely related to moisture content because the potential energy state is determined by conditions at the air-water interfaces and the nature of the surface films, rather than by the quantity of the water present in the pores. The welded tuff pores at Yucca Mountain are variable in size and shape and in the degree of interconnection. Jury et al. (1991 [DIRS 102010], p. 65) state that it is common for porous media to have bottleneck pores, in which there are large cavities but narrow points of connection to adjacent pores. Water is retained in small pores, which fill first when water is admitted to a system; however, they do not always empty again during drying in the same order as they were filled.

As the welded or nonwelded tuff is dried by evaporating water, pores will begin to empty from the state of near saturation in the tuff matrix. However, water may be trapped in the larger pore space in such a way that the pores will not empty in the order that they might be filled if water is introduced to dry welded tuff. The sudden release of a relatively large amount of water from a large pore floods surrounding pores and decreases the matrix potential in them temporarily. If matrix potential is measured in a small porous system having discrete differences in pore size, the relationship between moisture potential and moisture content for drying might be "saw toothed" (Jury et al. 1991 [DIRS 102010], Figure 2.14).

In welded tuff, the pore size distribution contains pores over a range of sizes, and the water and moisture potential distributions tend to average out so that a relatively smooth curve is obtained.

The moisture content for a given moisture potential is higher than for the wetting system, as shown by Jury et al. (1991 [DIRS 102010], Figure 2.14).

In addition, as discussed by Jury et al. (1991 [DIRS 102010]), surface wetting also introduces hysteresis. The grain surfaces will form a nonzero contact angle with water when wetted. This results in thicker films than would be present in the drying phase where water films are drawn tightly over the surface by adsorptive forces.

The conceptual model for water retention described above shows that the rates of imbibition generally would be overpredicted. The impacts of this overprediction would be an underprediction of temperature and an overprediction of relative humidity. Thus, the conceptual model suggests that liquid fluxes would be conservatively bounded, so determinations of the dryness of the waste package inner diameter will be conservative. However, waste package and drip shield temperatures would be nonconservatively bounded, which means that waste package and potential repository temperatures could exceed those calculated. As additional measurements characterize hysteresis properties in moisture retention in the matrix for welded and nonwelded tuffs, and in fractures for welded tuff, the uncertainty in temperatures will decrease.

5.3.1.4.4 Effects of Mountain-Scale Gas Phase Convection

Depending on its magnitude, the influence of mountain-scale and drift-scale buoyant gas-phase convection can influence MSTH model results in several ways. Buoyant gas-phase convection increases the rate of heat transfer away from the potential repository horizon and emplacement drifts. Therefore, if its magnitude is large enough, buoyant gas-phase convection will decrease temperatures in the host rock and in the emplacement drifts. For cases where boiling occurs, the decrease in temperatures can reduce the duration of boiling. Buoyant gas-phase convection can also increase the magnitude of heat-mobilized liquid-phase flux above the emplacement drifts.

To be significant to thermal-hydrologic conditions at the potential repository horizon, buoyant gas-phase convection requires thermally perturbed conditions arising from radioactive decay heat. The development of convection cells for layers heated from below depends on the critical Raleigh number. That dimensionless number is, in turn, proportional to the thermal expansion of the fluid, the temperature difference or gradient, and the intrinsic permeability (more specifically, the bulk permeability of the fracture continuum), and it is inversely proportional to thermal diffusivity and fluid viscosity (Phillips 1991 [DIRS 140641], pp. 144 to 145). Of these parameters, the several orders of magnitude range of variation of permeability has a more dominant effect on convection than thermal diffusivity which varies over a narrower range.

Sensitivity analyses were performed (Buscheck 2001 [DIRS 155243]) to consider a range of bulk permeability (k_b) values that incorporated plus or minus one (low-k_b and high-k_b) and two (very low-k_b and very high-k_b) standard deviations around the mean. For these analyses, the permeability distribution was isotropic. Since vertical anisotropy restricts buoyancy, the use of an isotropic permeability distribution provides an upper bound of the possible effects of buoyancy for any given value of permeability. Analyses by Phillips (1991 [DIRS 140641], p. 145) indicate that the critical Raleigh number is smaller when the ratio of permeability in the horizontal direction to the vertical direction is low, which may occur in some regions of the welded fractured units. The influence of vertical anisotropy is not directly addressed by the sensitivity analyses discussed in this section.

Figure 5.3.1.4.4-1 shows liquid flux calculations for the HTOM at 5 m above the drift for a central drift location. This location was chosen to be consistent with locations where seepage had been evaluated in past analyses (CRWMS M&O 2000 [DIRS 153363], Section 3.2.3.1.5). In the low-k_b case, these flux values represent the case in which buoyant gas-phase convection has a negligible influence on thermal-hydrologic behavior. The high-k_b case is more conducive for buoyant gas-phase convection to be significant. The mean k_b case is one in which the influence of buoyant gas-phase convection is modest, but not negligible. After about 20,000 years, there is no significant difference between the flux for the three cases. This indicates that the model results are not sensitive to considerations of buoyant gas-phase convection at late times when temperatures approach ambient conditions.

During the boiling period, the high-k_b case resulted in peak values of heat-mobilized flux above the emplacement drift being nearly twice those of the mean and low-k_b cases. These peak values occur during the early portion of the boiling period. This indicates that heat-mobilized liquid flux is sensitive to buoyant gas-phase convection during the early portion of the boiling period. The peak liquid flux for the high-k_b was 220 mm/yr, compared with 115 mm/yr for the mean and low-k_b cases. This indicates that heat-mobilized liquid flux is very sensitive to buoyant gas-phase convection during the early portion of the boiling period. The peak liquid flux for the high-k_b case was 220 mm/yr, compared with 115 mm/yr for the mean- and low-k_b cases. For cases in which the influence of buoyant gas-phase convection is negligible, the flow of heat-mobilized water vapor is vertically symmetric with respect to the potential repository horizon: about half flows above the potential repository horizon and about half flows below the potential repository horizon. When the influence of buoyant gas-phase convection is strong, it results in very pronounced vertical asymmetry of the water-vapor flow field, causing nearly all of the heat-mobilized vapor flow to occur above the potential repository horizon. This asymmetry in the water-vapor flow field causes the condensate flux above the potential repository horizon to be nearly twice that of the case where buoyant gas-phase convection is negligible.

Figure 5.3.1.4.4-2 shows the results for the LTOM analyses under the same conditions used in the HTOM analyses. The stairstep responses indicate the impacts of different climates from 0 to 600 years and from 600 to 2,000 years. Results for the LTOM do not show the significant differences between the low, mean, and high-k_b cases in contrast to the HTOM analyses from 1,000 to 2,000 years. This is mainly because, without boiling, there is much less water mobilized by vaporization and condensation. These analyses indicate the same long-term flux responses as the HTOM calculations: about 22 mm/yr, with a difference of less than 1 mm/yr among the low, mean, and high-k_b cases.

Heat mobilized liquid flux 5 m above the drift is more sensitive to buoyant gas-phase convection than it is at 1 m above the drift (compare Figure 5.5.1.4.4-3 with Figure 5.3.1.4.4-1). Analyses discussed in Section 5.3.1.4.2 indicate that seepage does not occur into drifts during the active boiling period. This is consistent with Figures 5.3.1.4.4-3 and 5.3.1.4.4-4 which show that there is no liquid flux 1 m above the drift in the HTOM case until after 700 years for the very-high and mean-k_b cases. At that point, the sensitivity to buoyant gas-phase convection is again apparent.

Around 1,000 years, there is greater flux in the very high-k_b case (52 mm/yr) than in the mean-k_b case (32 mm/yr), indicating some sensitivity of liquid flux to buoyant gas-phase convection. However, this amount of flux is about the same magnitude as the ambient flux range and less than the long-term flux from the wetter climates (up to 100 mm/yr). There is no significant difference in liquid-phase flux at 1-m and 5-m above the drift in the LTOM, reflecting the minimal thermal mobilization of water.

The influence of mountain-scale buoyant gas-phase convection on temperatures within the host rock and on the duration of boiling conditions was addressed in previous analyses (Buscheck et al. 1994 [DIRS 105157]). These analyses considered the impact of mountain-scale buoyant gas-phase convection on TH results for a number of different potential repository AML scenarios. Among the AMLs considered in those analyses was a 55.3-MTU/acre case that is comparable to the HTOM case AML (Table 5.1-1). The LTOM AML of 45.7 MTU/acre is bracketed by the 55.3 and 35.9-MTU/acre cases considered by Buscheck et al. (1994 [DIRS 105157]). Therefore, the results of the earlier analyses are adequate for evaluating uncertainties in the MSTH model results due to the effects of mountain-scale buoyant gas-phase convection and are discussed in the following paragraphs.

Buscheck et al. (1994 [DIRS 105157]) evaluated the effects of convection by considering values of bulk fracture permeability (k_b). As shown in Buscheck et al. (1994 [DIRS 105157], Table I), permeability ranged from sufficiently low (0.28 darcy) to limit convection (satisfying the critical Raleigh number) to a range (1 to 10 darcy) that is representative of the permeability range (and of the buoyant gas-phase convection effects) expected for the potential repository, and then to values that would represent the upper bounds (40 to 84 darcy) of permeability (1 darcy is approximately 10^{-12} m^2). The values of permeability used by Buscheck et al. (1994 [DIRS 105157]) are consistent with, the uncertainty and sensitivity analyses for this report. Specifically, the mean permeability value used in the MSTH model analyses for the lower lithophysal unit is 2.4 darcy which falls between the two values evaluated (1 and 10 darcy). Analyses of the sensitivity of MSTH model results to variability in k_b considered two standard deviations of k_b (see Section 5.3.1.4.7) about the mean. The upper value that represents two standard deviations (log scale) is 38.1 darcy, similar to the value of 40 darcy used by Buscheck et al. (1994 [DIRS 105157]). Thus, the 84-darcy case represents an extreme bound on the uncertainty. The lower value, two standard deviations, is 0.15 darcy. This is somewhat lower than the 0.28 darcy used by Buscheck et al. (1994 [DIRS 105157]). However, the 0.28 darcy case has a permeability that is sufficiently low that it does not generate significant mountain-scale buoyant gas-phase convection. A lower value would simply give the same non-convection results. Those analyses found, as did earlier analyses (Buscheck and Nitao 1994 [DIRS 130561]; Buscheck and Nitao 1993 [DIRS 140907]), that the permeability threshold where mountain-scale convection begins to dominate moisture movement is about 1 darcy.

The analysis (Buscheck et al. 1994 [DIRS 105157], Table I) evaluated the effect on peak temperature of neglecting convection (using 0.28 darcy as a negligible convection case). For a potential 55.3 AML repository (similar to the higher temperature operating mode), the peak temperature was reduced by 1.2, 3.7, and 5.2°C at 1 darcy (the most representative of the values used in current analyses), 10 darcy and 40 darcy respectively. The difference interpolated between these results to 2.4 darcy (the value for the lower lithophysal unit, in which most of the potential emplacement drifts would be located) is about 2°C. The analyses further indicated that there would be a difference of about 200 years in the duration of the temperature elevation above the boiling point for the lower lithophysal unit mean-k_b case and the 0.28-darcy case. This is based on differences in duration (from the 0.28 darcy case) of 60 years and 681 years for the 1 and 10 darcy cases, respectively. The same analyses indicate that for k_b of 40 darcy, about two standard deviations higher than the mean in the lower lithophysal unit, the peak temperature difference would be about 3°C lower than in the lower lithophysal unit mean-k_b case, and the difference in the duration of boiling would be reduced by more than a factor of two. Because these early analyses used no ventilation period, their duration of boiling is greater than expected in the potential repository.

The Buscheck et al. (1994 [DIRS 105157]) analyses performed for the 35.9 MTU/acre AML case are applicable, as a lower bound, to the LTOM case (45.7 MTU/acre) evaluated in this report. Those analyses found that for the 35.9 MTU/acre AML case, there was no difference in peak temperatures between the 0.28-darcy and 1-darcy cases, and only a 0.1°C difference between the 0.28-darcy and 10-darcy cases. If a linear interpolation to 2.4 darcy applies between the 35.9 and 55.3 MTU/acre AML cases, the temperature difference between the lower lithophysal unit mean-kb case and a permeability two standard deviations higher would be less than 1°C for an AML of 45 MTU/acre. If a linear interpolation of peak temperature is used between the 35.9 and 55.3 MTU/acre AML cases, the 45-MTU/acre case would peak at about 96°C, just at the boiling point of water at the potential repository elevation and there would be no duration above boiling.

Summary-The primary effect of neglecting mountain-scale gas-phase convection occurs on the potential repository temperatures and the duration of boiling. Based on the results of the studies described above, it can be concluded that neglecting mountain-scale buoyant gas-phase convection in the MSTH model analyses will conservatively bound temperatures on the high side. For the HTOM, the calculated temperatures would be less than 2°C too high for the mean-k_b case. A permeability two standard deviations higher than the mean would produce temperatures about 1° and 3°C higher than actual for the lower and higher-temperature operating modes, respectively.

5.3.1.4.5 Effects of Thermal-Hydrologic-Chemical Processes

Changes in porosity and permeability from mineral dissolution and precipitation have the potential to modify percolation fluxes and seepage fluxes at the drift wall. Porosity changes in matrix and fractures are directly tied to volume changes as a result of mineral precipitation and dissolution. Since the molar volumes of minerals created by hydrolysis reactions (i.e., anhydrous phases, such as feldspars, reacting with aqueous fluids to form hydrous minerals, such as zeolites or clays) are often larger than those of the primary reactant minerals, dissolution-precipitation reactions can lead to porosity reductions. This section summarizes an analysis (BSC 2001 [DIRS 154677]) of the effects of THC coupled processes.

As noted in Section 5.3.1.2.2, the TSPA-SR (CRWMS M&O 2000 [DIRS 153246] was supported by analyses that indicated that THC processes would not have a significant impact on hydrologic properties. These analyses are documented in *Drift-Scale Coupled Processes (DST and THC Seepage) Models* (BSC 2001 [DIRS 154677]; see also Sections 4.3.6.3.2 and 4.3.6.4.2 of this document). Fracture permeability changes can be approximated using the porosity change and an assumption of plane parallel fractures of uniform aperture (Steefel and Lasaga 1994 [DIRS 101480], p. 556). However, this approximation yields a permeability of zero only for a zero fracture porosity. In many experimental and natural systems, permeability reductions to values near zero occur at porosity significantly greater than zero. This is usually the result of mineral precipitation or fracture closure of the narrower interconnecting apertures. The hydraulic aperture, as calculated from fracture spacing and permeability (determined through air-permeability measurements) assuming a cubic law relation, is a closer measure of the smaller apertures in the flow system. These analyses used the hydraulic aperture.

Analyses documented in *Drift-Scale Coupled Processes (DST and THC Seepage) Models* (BSC 2001 [DIRS 154677] Section 7) concluded that predicted porosity changes due to water-rock interaction around waste emplacement drifts are small and show a reduction mostly due to mineral precipitation, with essentially no effect on predicted thermal-hydrologic conditions around drifts. The Tptpmn THC backfill model predicted small fracture porosity changes due to mineral precipitation and a small effect of porosity changes on permeability. Depending on the infiltration rate, the largest fracture porosity reductions occurred approximately 15 to 18 m above and to the side of the drift (BSC 2001 [DIRS 154677] Section 6.3.4 and Figure 52). The predicted reduction in porosity and permeability in the NFE over 100,000 years for the Tptpmn (no backfill and homogeneous permeability) is less than 3 percent of the initial fracture porosity and less than one order of magnitude, respectively. This is somewhat greater than calculated for the Tptpmn THC backfill model (less than 1-percent change in fracture porosity), but still relatively minor.

These results (BSC 2001 [DIRS 154677], Section 7) are based on uniform areas of precipitation in plane parallel fractures; the actual effects in heterogeneous fractures with rough surfaces and nonuniform mineral precipitation may be greater. The analysis does not account for the effects of anisotropy in the fracture permeabilities. Comparison of the results of purely thermal-hydrologic simulations to those including coupled THC processes show only small differences in predicted water and gas fluxes, liquid saturation, and permeability around the drift. The porosity reduction that occurs well after rewetting of the drift wall is predicted to be almost entirely due to calcite and amorphous silica. The latter contributes to most of the initial precipitation during the initial cooling stage, with maximum deposition spreading above the drift in a zone roughly coinciding with the maximum extent of the dryout zone (8 to 10 m from the drift center). Dissolution of salts is expected to occur during this stage, but the effect on fracture porosity and permeability is negligible. Calcite is predicted to precipitate mostly during later cooling stages. During the cooling stages, amorphous silica dissolves slightly, as do some primary minerals, such as feldspars; however, this dissolution is not sufficient to reverse the porosity reduction that occurs due to precipitation (BSC 2001 [DIRS 154677]). Below the drift, little mineral alteration takes place during heating and cooling because of the drift shadow effect, resulting in a region sheltered from infiltrating water.

The analyses (BSC 2001 [DIRS 154677], Section 7) further concluded that heterogeneity in fracture permeability can have varied effects on thermal hydrology, including flow focusing and irregularity in isotherms and liquid saturations. TH simulations were performed for three heterogeneous fracture permeability realizations with a range in permeability of four orders of magnitude, under the mean infiltration climate change scenario, for the Tptpmn unit. Areas of highest initial liquid saturation, which have lower permeability and generally reside above the drift, tend to show the greatest reduction in fracture permeability, down to about 25 percent of the initial value in some regions. This localized permeability reduction tends to cause some additional flow focusing, but the permeability changes are considerably less than the initial range in permeability. The corresponding maximum fracture porosity reductions are approximately 5 percent of the initial value.

Porosity reductions (BSC 2001 [DIRS 154677], Section 7) for the extended geochemical system are slightly greater than those for the base case system owing to more mineral species precipitating and somewhat higher silica concentrations in the former. The maximum amount of amorphous silica precipitated is about 2 percent (volume percent of fracture) in the extended case and somewhat less in the base case, with maximum amounts in the high saturation zones near the drift.

Because of the large amount of data needed and the complexity of natural systems, many uncertainties exist in modeling coupled THC processes (BSC 2001 [DIRS 154677], Section 7). The necessary data include the fundamental thermodynamic properties of minerals, aqueous species, and gases; the kinetic data for mineral-water reactions; and the representation of the unsaturated hydrologic system for fractured tuffs. In addition, site-specific thermal-hydrologic, geologic, and geochemical data are necessary to describe the initial and boundary conditions. For these reasons, it may not be possible to assign a model uncertainty based on the uncertainties of the data themselves; therefore, model validation gives a true test of whether the system can be described sufficiently well for the intended purposes of the model.

A comparison of simulated THC processes to those processes measured during the Drift Scale Test was conducted (BSC 2001 [DIRS 154677], Section 6.2). It was found that the simulations captured the important changes in pH, aqueous species concentrations, and gas-phase carbon dioxide concentrations at specific locations over time. This provides sufficient validation of the capability of the model to predict spatial and temporal variation in water and gas chemistry.

5.3.1.4.6 Effects of Thermal-Hydrologic-Mechanical Processes on Multiscale Thermal-Hydrologic Model Results

The influence of uncertainty on TSPA-SR results relates to whether ignoring THM effects, as the current models do, can significantly affect MSTH model results. The THM effects addressed in this section are those related to hydrologic effects, specifically changes in permeability. While fracture aperture changes due to THM effects may influence the water retention potential of fractures, no attempt has been made to address these processes other than the correlation between permeability and van Genuchten α discussed in Section 5.3.1.4.2. As noted in Sections 5.3.1.4.8 and 5.3.1.4.9, porosity influences thermal conductivity. However, the fracture porosity (about 1 percent; see Section 4.3.6.3.2) is less than 10 percent of the total porosity (see Section 5.3.1.4.9 for lithophysal porosity values). Changes in that 10 percent will not have as significant an effect on thermal conductivity as changes in the matrix and lithophysal porosity. THM may also influence convective heat transfer by causing changes in the permeability of the fractures. Section 5.3.1.4.4 addresses the sensitivity of the MSTH thermal model results to mountain-scale convection; this section focuses entirely on THM-induced changes in permeability that could be the cause of such convection.

Analyses of THM effects on hydrologic properties, specifically on fracture permeability, are reported in the *Near Field Environment Process Model Report* (CRWMS M&O 2000 [DIRS 153363], Section 3.5). The analyses used a distinct element model to represent fracture-bounded blocks. The analyses identified a potential for localized increases in permeability of up to a factor of six. The changes were based on predicted shear displacements and an empirical relationship between displacement and permeability change.

More recent work evaluated permeability changes due to both normal and shear deformations (Blair 2001 [DIRS 155005]). In this work, the model boundaries were extended horizontally to the mid-pillar region on either side of the drift and vertically to 100 m above and below the emplacement drift, but the fractured region remained relatively small at $20 \times 20 \times 10$ m due to computational limitations. A fixed stress boundary condition, equivalent to the weight of the overburden, was applied to the upper boundary, and fixed displacement boundary conditions were applied to the sides and lower boundary. Shear deformations were assumed to increase fracture apertures as mismatched fracture surfaces slide past each other so that the cubic law could be used to assess permeability changes resulting from shear as well as normal deformations. All fractures were assumed to have the same initial aperture. The predicted permeability changes are quite sensitive to aperture changes because of the cubic law, so that the initial fracture aperture used in the simulations is expected to affect the model results. Model input parameters are given in Table 5.3.1.4.6-1.

Heating was found to cause a rotation of the stress field at the level of the emplacement drift. The maximum principal stress rotated from vertical to horizontal during the heating period, then rotated back to vertical by 100,000 years as the rock cooled. The rotation of the local stress field closed subvertical fractures and opened subhorizontal fractures during the heating period. In the HTOM case, permeability decreased by five to six orders of magnitude in 80 percent of the subvertical fractures, and by lesser amounts in most of the other subvertical fractures, by 100 years into heating. The five order of magnitude reduction in permeability persisted until at least 1,000 years for 70 percent or more of the subvertical fractures. Over the same time interval, permeability increased by up to one order of magnitude in 20 to 45 percent of the subhorizontal fractures and remained little changed in most of the rest. Predicted permeabilities increased for all fractures during cool-down, generally by one or two orders of magnitude. The THM effects are concentrated at the emplacement drift level where the temperature perturbations are greatest. The rock a few drift diameters above and below the emplacement drift level will likely experience more modest THM-induced permeability changes because the temperature changes are smaller.

The LTOM case was analyzed and results show that as expected, the stress levels in the rock mass are much lower than for the HTOM case, and that the highest stresses occur after the end of ventilation at 300 years after emplacement. In addition, the results show that for the LTOM the fracture permeability remains basically unchanged for the first 300 years of storage while ventilation is maintained. Results also show that after the end of the ventilation period (300 yr) a decrease in fracture permeability of one to two orders of magnitude is predicted for approximately 50 percent of the vertical fractures. This reduction of fracture permeability is predicted to persist until 400 years after emplacement, and gradually changes over time, with fracture permeability decreasing by 3 orders of magnitude in approximately 20 percent of the vertical fractures at 1,000 years after heating.

While the predicted decreases in fracture permeability due to TM effects after the end of the ventilation period may be significant for the LTOM case, they are much smaller in magnitude and affect far fewer fractures than the changes in fracture permeability predicted for the HTOM case. THM modeling results for both the HTOM and LTOM cases are discussed in detail in Section 4.3.7.

The analyses of thermal-hydrologic sensitivity to bulk permeability (see Section 5.3.1.4.7) considered a range of permeabilities, as shown in the first three columns of Table 5.3.1.4.6-2. The seepage analyses described in Section 5.3.1.4.2 also considered a range of permeabilities and the effects of heterogeneity. Table 5.3.1.4.6-2 reports the ranges considered for heterogeneous fracture permeability without strong vertical focusing in the seepage sensitivity studies (Table 5.3.1.4.2-1, Case A) because this range is more constrained than the extreme cases. In Table 5.3.1.4.6-2, the ranges evaluated in Sections 5.3.1.4.2 and 5.3.1.4.7 are compared with potential changes in permeabilities due to shear displacement (increases) and normal displacements (decreases). These changes, shown in the last column of the table, were calculated by applying the order of magnitude increase and five orders of magnitude decrease to the mean permeability values listed in the first column of the table for units tsw34 and tsw35. Although the magnitude of THM changes only applies to regions near the drift (i.e., to the tsw34 and tsw35 units that constitute most of the potential repository horizon (BSC 2001 [DIRS 155010]). The upper bound is based on the one order of magnitude increase in permeability found for a substantial number of subhorizontal fractures during the heating phase of the THM model. The lower bound is based on the five order of magnitude drop in permeability during the heating phase for subvertical fractures. At later times, after a significant amount of cooling has occurred, a higher permeability bound of two or three orders of magnitude at the drift elevation is appropriate based on the THM results. Changes of these magnitudes only apply to the near-drift environment (i.e., to the TSw34 and TSw35 units that constitute the potential repository horizon). The thermal-mechanical effects depend on temperature changes that will be progressively less pronounced away from the drift level, but can be considered to form a loose upper bound on the potential THM influence on the permeability of the other units.

The range of possible changes in permeability due to THM processes (Table 5.3.1.4.6-2, column 5) was compared with permeability variability/uncertainty ranges used in the sensitivity analyses discussed in Sections 5.3.1.4.2 and 5.3.1.4.7 (Table 5.3.1.4.6-2, columns 3 and 4). The range of increased permeabilities due to THM was smaller than the range considered in the permeability sensitivity analyses. However, reductions in permeability along vertical fractures predicted by the THM analysis were greater than those considered in the sensitivity analyses. As noted in Section 5.3.1.4.7, there was no difference between the mean- and low-k_b analyses in temperatures or relative humidities on the drip shield or the drift wall. This would indicate that, although THM effects reduced the permeability below the low k_b values, the model results would not be affected. Normal deformations would diminish with decreased temperature changes. The maximum decreases in permeability due to normal displacement take place at 100 years, then gradually decrease with time (Blair 2001 [DIRS 155005], Section 6.3.3). For the HTOM, it appears that the sensitivity analyses of temperature and relative humidity effects are applicable to the ranges of possible permeability changes from THM processes. Therefore, neglecting changes in permeability due to THM effects will have a range of effects on MSTH model results those discussed in Sections 5.3.1.4.2 and 5.3.1.4.7.

Changes to the upper or lower, rather than the mean values of the permeability could be beyond the ranges evaluated in the seepage and bulk permeability analyses. If the lower values are decreased, the effect will be to hinder liquid as well as vapor flow. If the upper values are decreased, the changes will be closer to the ranges evaluated in Sections 5.3.1.4.2 and 5.3.1.4.7. If THM processes cause increases to the upper permeability values, large-scale buoyant gas-phase convection could be promoted and the effects will be beyond those evaluated in (Section 5.3.1.4.4). However, the THM model predicts contrasting changes in permeability during the heating phase, with vertical permeability generally declining by a greater margin than horizontal permeability increases, so that increased large-scale convection is doubtful. It can also be argued that higher permeability fractures do not impede vapor or water flow, so increases are not likely to result in major differences in MSTH model temperature results. This is supported by analyses of the influence of permeability range on the MSTH model. As noted in Section 5.3.1.4.7, after 1,000 years the temperatures on the drift wall and drip shield are insensitive to the range of permeability evaluated. At earlier times, the most significant difference was in the HTOM, for which the temperature was about 2° to 4°C lower in the high case during the first 50 years. The relative humidity results for the drip shield were insensitive to the permeabilities, and the results for the drift wall were nearly insensitive to permeabilities, with a difference of less than 1-percent between the high k_b results and the mean and low k_b results. Thus, it is concluded that THM induced increases to lower-bound permeability values will result in permeabilities and TH effects within the bounds addressed in previous sensitivity analyses. For THM changes to upper-bound permeabilities, the seepage analyses for Case-D fractures considered larger-than-normal heterogeneities (2.3 log k sigmas) (see Section 5.3.1.4.2). Although these analyses would be more applicable to the extreme cases, they would not cover THM changes of five orders of magnitude.

The most significant uncertainty regarding the THM results is probably due to model and process uncertainties rather than input data uncertainties. Because of the convolution of model and process uncertainty, the approach used to date to evaluate the impacts of uncertainty has been to compare model analyses with field tests. Although these comparisons do not provide quantification or direct evaluation of the uncertainties, they do allow for an assessment of whether the model results are realistic. The remainder of this section focuses on comparisons of model results with measurements at the Large Block Test (CRWMS M&O 2000 [DIRS 153363], Section 3.6.1.1).

Deformation of the large block during the test was monitored using multiple-point-borehole-extensometers, and a distinct element code (3DEC V2.0) was used to simulate TM behavior. The distinct element method was chosen because it allows discrete fractures to be incorporated into the simulation. The TM model attempts to predict fracture displacements, which are thought to control permeability changes in the tuff. Accurately modeling fracture displacements is a necessary (but not sufficient) condition for modeling THM processes in a realistic manner. Deformation of the large block was calculated at eighteen times of between the start of the test up to 450 days after the start of heating. The model temperatures were derived from the TH analysis performed using submodels of the MSTH model and documented in the *Thermal Tests Thermal-Hydrological Analyses/Model Report* (CRWMS M&O 2000 [DIRS 151964], Section 6.4.3).

A series of simulations (Blair 2001 [DIRS 155309]) was conducted to evaluate the effects of the number of fractures in the model and the coefficient of thermal expansion. These simulations are listed in Table 5.3.1.4.6-3, and the geometry of the model domain for the various simulations is shown in Figure 5.3.1.4.6-1.

The multiple-point-borehole-extensometers in borehole WM2 functioned well throughout the test, and data from anchor WM2-4 representing the entire WM2 baseline comprise the best available basis for comparing model displacements with field data (Figure 5.3.1.4.6-2). The model simulations differ only in the number of fractures or the thermal expansion coefficient. Model 1, the continuum model, incorporates no fractures. Model 2 includes the six largest fractures, and incorporates a higher thermal expansion coefficient than the other models. Models 3 and 4 incorporate only the six and seven largest fractures respectively, while Model 5 includes more than twenty additional, smaller fractures.

Models 3 and 4 did a good job of predicting the deformation at anchor WM2-4 over much of the test duration, including both the heating and cooling phases (Figure 5.3.1.4.6.2). Model 3 predicts slightly less displacement than Model 4. Models 3 and 4 underpredict the total displacement during cooldown by 0.4 mm, and they predict some contraction of the block at about 270 days that is not reflected by observations. Model 1 (continuum) and Model 5 (many fractures) both underpredict the maximum deformation by significant amounts (1.6 and 1 mm, respectively). Model 2 (high coefficient of thermal expansion) overpredicts the maximum deformation, but it shows the best fit to displacement during the first 20 days of heating. Model 5 (many fractures) does not show contraction with cooldown, and Model 1 (continuum) underpredicts the magnitude of the cooldown displacement. Model 2 (high coefficient of thermal expansion) correctly predicts the relative change in displacement during cooldown (1.8 mm), but the final displacement value of 2.6 mm is too high.

Results from the Large Block Test indicate that the distinct element model predicts deformation behavior more accurately than the continuum model. Moreover, not all fractures were active; the deformation was controlled by a subset of 6 to 10 major fractures. Modeling results also indicate that a coefficient of thermal expansion value of 5.27×10^{-6} °C is appropriate for the Large Block Test. This is lower than the value measured on laboratory samples, but consistent with the value determined from deformation measurements in the Single Heater Test (CRWMS M&O 2000 [DIRS 153363], Section 3.6.1.2) conducted in the ESF. Although the Large Block Test model simulations were not used to predict changes in permeability or moisture retention, simulations that fail to account correctly for fracture displacements likely will fail to predict changes in permeability and other hydrologic properties related to fracture aperture.

Summary–The influence of THM processes on permeability is generally within the range of the seepage and bulk permeability effects reported in Sections 5.3.1.4.2 and 5.3.1.4.7, respectively, for the upper bounds of permeability. Increases in the upper permeability bounds may promote buoyant gas-phase convection (Section 5.3.1.4.4). The decreases in the lower permeability values by as much as five orders of magnitude are beyond the ranges investigated in the permeability sensitivity studies; however, it does not appear that these changes will significantly affect temperature or relative humidity. The decrease in vertical permeability should reduce seepage into the drifts, although this effect will be at least partially offset by the re-opening of vertical fractures during cooldown. Based on these assessments, it is concluded that the uncertainties from neglecting THM within the MSTH models will not increase those addressed in the sensitivity studies for the HTOM.

5.3.1.4.7 Sensitivity to Host Rock Bulk Permeability

Sensitivity analyses were performed to consider the impacts of uncertainties in the values of fracture permeability used in the MSTH model. In the MSTH model, fracture and matrix are handled as the separate but overlapping continua (dual-permeability model) in which the permeability of the matrix and the fractures are expressed as different bulk permeabilities applied uniformly to the rock mass. Since the actual fracture permeability is heterogeneous, applying a bulk permeability to the heterogeneous system could introduce uncertainties in the results. Because the fracture permeability rather than the matrix permeability (which is significantly smaller) dominates the TH processes, the practice has been to refer to the bulk permeability (k_b) without distinguishing between the matrix and fracture permeability. Thus, the term "bulk permeability" actually refers to the bulk fracture permeability. This practice will be followed throughout this section.

Sensitivity analyses (Buscheck 2001 [DIRS 155243]) were designed to address the potential for impacts by comparing the results over a wide range of fracture properties. The first analysis considered the impacts that a range of k_b representing approximately one standard deviation above and below the mean values (identified as high, mean, and low k_b) had on both temperatures and relative humidity on the drift wall and drip shield in the center of the potential repository (CRWMS M&O 2000 [DIRS 149862)], Figure 5-2, location L5C3) for the HTOM with the mean infiltration flux. Analyses were also conducted for two standard deviations above and below the mean values (identified as very high, mean, and very low k_b). Although the analyses were for the L5C3 location, they are applicable to the portion of the potential repository in which the host rock is the Tptpll unit, which comprises more than three-quarters of the potential repository area. The actual values for k_b used in determining the very high, high, mean, low, and very low k_b values in the models are shown in Table 5.3.1.4.7-1. As can be observed in Figure 5.3.1.4.7-1, the temperatures beyond 1,000 years on the drift wall and the drip shield were insensitive to the k_b used in the models for the HTOM. A few decades after closure there was some sensitivity of drift wall and drip shield temperature to bulk permeability. The drift wall temperatures were consistent for the mean and low k_b cases, but slightly higher than the temperature for the high k_b case. The drip shield temperatures were not sensitive to differences between mean and low k_b, while the high k_b resulted in a slightly lower temperature. For the very high and high k_b cases, the peak temperature is 11°C and a few °C lower, respectively than in the mean k_b, low k_b, and very low k_b cases.

The relative humidity results for the drip shield (Figure 5.3.1.4.7-1) were insensitive to the k_b and nearly insensitive for the drift wall; there was less than a 1-percent difference among the five cases. The results suggest that for the mean infiltration case, the MSTH model relative humidity results for the drift wall and drip shield are relatively insensitive to repository-scale permeability variability. This indicates that repository-scale variability of k_b will not significantly modify MSTH model predictions of temperature and relative humidity in portions of the potential repository for which the Tptpll is the host rock unit. The weak dependence of temperature and relative humidity on k_b in the Tptpll unit indicates that temperature and relative humidity predictions by the MSTH model would also be relatively insensitive to k_b in portions of the potential repository where the host-rock unit is other than the Tptpll.

Sensitivity of the MSTH model liquid saturation in the invert material was also evaluated. Figure 5.3.1.4.7-2 shows the predicted liquid saturation in the higher-temperature operating model for the same location within the potential repository footprint as the temperature and relative humidity assessments discussed above. The results are for the upper invert layer directly below the drip shield in the central portion of the drift (Figure 5.3.2.3-1 shows the computational cells in the invert). The index i in Figure 5.3.1.4.7-2 is 4 for the outermost invert cell and 1 for the innermost cell. These analyses were performed for the mean infiltration flux case.

Figure 5.3.1.4.7-2 shows that the liquid saturation in the upper invert is zero until about 2,000 years after emplacement for the mean and low k_b cases and about 3,000 years for the high k_b case (Figure 5.3.1.4.7-2). The very high k_b case has an onset of rewetting at about 4,000 years. The general trend from these five permeability cases is that the onset of rewetting increases with k_b and that the final "steady-state" value of liquid saturation increases with decreasing permeability. As the permeability decreases, liquid saturation in the fractures must increase to accommodate a given percolation flux; the increased liquid saturation results in lower capillary tension in the fractures and adjoining rock matrix. The lower capillary tension in the host rock promotes more wicking of moisture into the crushed-tuff invert. Because the capillary properties of the fractures were not varied along with the permeability and because a single continuum was used to represent the crushed-tuff invert, the trend between these permeability cases should be viewed qualitatively rather than quantitatively.

A similar set of analyses was performed for the LTOM. These analyses considered the same range of permeability and the same location within the potential repository footprint as can be observed in Figure 5.3.1.4.7-3; the temperatures on the drift wall and the drip shield are insensitive to the k_b bulk permeability used in the models. The relative humidity on the drip shield and drift wall is also insensitive to the permeability. This indicates that repository-scale variability of permeability will not significantly modify MSTH model predictions of temperature and relative humidity in portions of the potential repository for which the Tptpll is the host rock unit. The weak dependence of temperature and relative humidity on permeability also indicates that temperature and relative humidity predictions by the MSTH model would also be relatively insensitive to permeability in portions of the potential repository where the host-rock unit is other than the Tptpll.

The relative humidity of the drift wall for the LTOM is always nearly 100 percent (which is the relative humidity for ambient conditions), whereas for the HTOM, relative humidity drops to 20 percent about 10 years after closure and then gradually increases with time until it reaches nearly 100 percent around 1,000 years after emplacement; thus, relative humidity at the drift requires about 1,000 years to return to ambient conditions. For this reason, the results of the MSTH model are not only insensitive to variations in k_b of two standard deviations about the mean, but are also conservatively bounded in the maximum relative humidity for this lower temperature operating mode. If there are any effects on the results from permeability much different from the mean permeability value (e.g., due to capillary effects), the results could only reduce the relative humidity. Because relative humidity effects performance at higher values, the results of the MSTH model provide a conservative bound.

The sensitivity of the MSTH model liquid saturation in the invert material was also evaluated for the LTOM. Figure 5.3.1.4.7-4 shows the predicted liquid saturation at the same location in the potential repository footprint as the temperature and relative humidity assessments discussed above. The results are for the upper invert layer directly below the drip shield, in the central portion of the drift (Figure 5.3.2.3-1). These analyses were performed for the mean infiltration flux case. The onset of rewetting occurs earlier in the invert for the LTOM than for the HTOM (compare Figures 5.3.1.4.7-4 and 5.3.1.4.7-2). The same trends between the permeability cases are observed in the LTOM as in the HTOM. The general trend is that the onset of rewetting increases with permeability and that the final "steady-state" value of liquid saturation increases with decreasing permeability. Because the capillary properties of the fractures were not varied along with the permeability of the fractures and because a single continuum was used to represent the crushed-tuff invert, the trend between these k_b cases should be viewed qualitatively rather than quantitatively.

Comparison of Results of Higher- and Lower-Temperature Operating Modes-Peak temperatures on the drift wall in the central portion of the potential repository for the HTOM and the LTOM are about 144 and 74°C, respectively; under mean infiltration and mean permeability conditions for the MSTH submodel. The temperatures decrease to ambient (i.e., approximately 22.5°C for the glacial climate) around 100,000 years. The relative humidity on the drift wall for the HTOM drops to about 20 percent about 10 years after closure, then increases to nearly 100 percent at about 1,000 years. The temperatures at the time that the drift wall relative humidity approaches 100 percent are about 90°C, and decrease to 70°C around 4,000 years. Thus, there is a period of about 3,000 years when the relative humidity is nearly 100 percent and temperatures are higher than 70°C. For the LTOM, the relative humidity is always nearly 100 percent. The drift wall temperatures for the LTOM are between 70 and 74°C from about 400 to 1,500 years. Thus, there is a period of about 900 years when the temperatures are slightly above 70°C and the relative humidity is nearly 100 percent.

Summary-Uncertainty in the values of bulk permeability that were used as inputs to the MSTH model, as evaluated in the sensitivity studies of two standard deviations from the mean value, had very little effect on the temperature and relative humidity at the drift wall and drip shield for the HTOM and LTOM. Liquid saturation in the invert has the same weak dependence on bulk permeability for the HTOM and the LTOM. The general trend is that the onset of rewetting increases with permeability and that the final "steady-state" value of liquid saturation increases with decreasing permeability. Because the capillary properties of the fractures were not varied along with the k_b of the fractures and because a single continuum was used to represent the crushed-tuff invert, the trend between these k_b cases should be viewed qualitatively rather than quantitatively.

5.3.1.4.8 Sensitivity to Host Rock Thermal Conductivity

Sensitivity analyses were performed to consider the uncertainties in drift-wall and drip-shield temperature, and relative humidity, and invert liquid saturation that result from uncertainties in the values of host rock thermal conductivity used in the MSTH model. Section 5.3.1.4.11 discusses the Waste Package temperatures and relative humidities. The MSTH model uses values of bulk host rock thermal conductivity as input. In field and laboratory measurements of host-rock thermal conductivity used in these thermal-hydrologic calculations, there is not discrimination between the relative contributions of the fractures and matrix to the bulk thermal conductivity. However, it is recognized that fractures and void spaces can have a significant impact on the thermal conductivity. It has been also recognized (CRWMS M&O 2000 [DIRS 149862], Sections 4.1.7 and 5.2.4) that there is a significant difference in thermal conductivity between wet (or saturated) rock and dry (or unsaturated) rock. The liquid saturation state of the rock mass must be determined by the MSTH model analyses for any given time. Therefore, there are uncertainties in the value of thermal conductivity to use, which could introduce uncertainties in the MSTH model results.

The calculation *Thermal Conductivity Properties for the Tptpll and Tptpul* (BSC 2001 [DIRS 155008]) was performed to estimate the range of matrix and rock mass thermal conductivity under various states of saturation in the lower lithophysal zone of the Topopah Spring unit (Tptpll), which accounts for variability in matrix properties, and in larger-scale features. For the lower lithophysal unit, the thermal conductivity data are limited to only several samples. Therefore, predictive relations were evaluated for application with matrix properties from several boreholes and rock mass properties from Enhanced Characterization of the Repository Block (ECRB) mapping and borehole geophysics measurements to provide a range of thermal conductivity based upon more abundant data on matrix properties.

The Kunii and Smith predictive relation (Kunii and Smith 1960 [DIRS 153166], p. 75) provides a method for predicting the stagnant thermal conductivity based upon matrix porosity, the thermal conductivity of the solids, and the thermal conductivity of the fluid (air or water) for porous rocks. Two bounding relationships were also considered for parallel flow and series flow (Hadley 1986 [DIRS 153165], p. 914). An evaluation of these relationships was made under the assumption of constant mineralogy and uniform thermal conductivity within these units. This assumption is reasonable given the small changes in grain density that are observed for these units (Rautman and Engstrom 1996 [DIRS 101008], p. 28).

The thermal conductivity of the rock mass for the Tptpll unit was estimated based upon an evaluation of the lithophysal porosity using two different methods. The first method used the information from mapping the ECRB drift (Mongano et al. 1999 [DIRS 149850]). The second method used information from core data and bulk density from geophysical measurements for borehole USW SD-7 at Yucca Mountain (BSC 2001 [DIRS 155008]). The porosity estimates from descriptive statistics of the ECRB mapping and the calculation of the lithophysal porosity from borehole USW SD-7 are comparable, and show that the mean values for lithophysal porosity are 0.125 and 0.120, respectively (see Section 4.3.5.3.2). The second method showed a low degree of correlation among the parameters of matrix saturation, matrix porosity, and air-filled lithophysal porosity.

The Monte Carlo simulation method (Hahn and Shapiro 1967 [DIRS 146529], pp. 237 to 241) was used to calculate expectation and variance of thermal conductivity for the Kunii and Smith (1960 [DIRS 153166], p. 75) predictive relation, the parallel predictive relation, and a composite predictive relation. The composite predictive relation uses the Kunii and Smith predictive relation for matrix properties and the parallel predictive relation (Hadley 1986 [DIRS 153165], p. 914) for the air-filled lithophysal porosity. The results of these calculations for the Tptpll unit (BSC 2001 [DIRS 155008], Section 6) are shown as the high and low cases in Table 5.3.1.4.8-1.

Sass et al. (1988 [DIRS 100644], p. 35) conducted a heat flow investigation for borehole USW G-4 located at Yucca Mountain, which was based upon a large number of measured thermal conductivities and a profile obtained in water-filled casing. This information can be used to determine if the predicted changes in thermal conductivity between the Tptpmn and the Tptpll units, based upon the composite model presented above, are reasonable. Sass et al. quotes a value for the average thermal conductivity of 2.02 W/(m K) based upon 13 samples of densely welded tuff in USW G-4. Between depths of 150 and 400 m, Sass et al. found that the gradient averaged 17.8 ± 0.04°C/km. The calculated heat flux rate was 36 ± 1 mW/m^2. A second calculation was performed below 400 m, where an abrupt increase in thermal gradient was observed. The thermal gradient increased to 30.1 ± 0.06°C/km, which is nearly twice the observed gradient at this depth. Considering the thermal conductivity of the Calico Hills to be 1.07 ± 0.04 W/(m K), substitution into Equation 1 (Sass et al. 1988 [DIRS 100644], p. 35) yields 32 mW/m^2. Sass et al. concluded that given the numerous sources of possible error, the agreement between these two independent heat flow determinations was excellent, and that heat flow in the UZ is primarily by heat conduction.

The same technical approach (BSC 2001 [DIRS 155008], Section 6, Figure 34) was adopted for evaluation of the thermal gradients between the Tptpmn and the Tptpll units for borehole USW G-4. The composite predictive relation presented above was found to be in better agreement with the geophysical measurements of temperature gradients in borehole USW G-4 (DTN: GS960708312132.002 [DIRS 113584]) than other models investigated.

Using the values of thermal conductivity determined in the analyses described above (BSC 2001 [DIRS 155008]), the MSTH model sensitivity analyses (Buscheck 2001 [DIRS 155243]) using the LDTH Submodel were designed to address the potential for impacts of uncertainty in thermal conductivity by comparing the results of analyses over the range of thermal conductivity values determined. Table 5.3.1.4.8-1 reports the values of thermal conductivity used in the models. The high and low values represent those determined by the Monte Carlo simulations and the mean determined from the ECRB measurements, geophysical measurements, and analyses of Sass et al. (1988 [DIRS 100644]).

The first set of sensitivity analyses considered the HTOM impacts. These analyses evaluated that the range of conductivity (the high, mean, and low conductivities shown in Table 5.3.1.4.8-1) had on temperature and relative humidity on the drift wall and the drip shield for a location in the center of the potential repository (CRWMS M&O 2000 [DIRS 149862], Figure 5-2, location L5C3) for the HTOM case with the mean infiltration flux. Although the analyses were for the L5C3 location, they are applicable to the portion of the potential repository in which the host rock is the Tptpll unit, which comprises more than three-quarters of the potential repository area.

Temperatures on the drift wall and drip shield are sensitive to the thermal conductivity (K_{th}) used in the models for as long as 100,000 years (Figures 5.3.1.4.8-1a and 5.3.1.4.8-1b). The MSTH model temperature results are more sensitive to variability in K_{th} values represented by values lower than the mean than they were to values above the mean. The drift wall peak temperatures for the low K_{th} values are nearly 220°C, compared to almost 150°C for the mean. The difference was around 70°C, which was almost 50 percent higher than the mean value temperatures. The difference between the mean and high K_{th} temperatures was much less (about 12°C): 136°C for the high K_{th} compared to 148°C for the mean value, which is only 5 percent lower than the temperatures for the mean value. At 1,000 years after emplacement, the difference between the mean and high K_{th} results is negligible (2° to 3°C), with the mean K_{th} temperatures around 96 to 97°C, the boiling temperature of water. This is significant, since at 1,000 years the low K_{th} temperatures are 112°C and rock at the drift wall would remain above the boiling point for approximately another 1,000 years.

Similar sensitivity to the K_{th} values used in the MSTH model analyses was observed in temperatures on the drip shield. The peak temperature for the low K_{th} was 234°C, compared to 160°C for the mean and 150°C for the high K_{th} values. The differences between the mean calculation results and the low and high K_{th} calculation results are 46 percent and 6 percent, respectively. Again, the differences persist for up to 100,000 years, while the difference between the mean and high K_{th} results essentially become insignificant within about 1,000 years. The temperatures drop to the boiling point at about the same time as the drift wall temperatures (approximately 1,500 years and 2,000 years for the mean/high and low K_{th} values, respectively).

There are significant differences in calculated relative humidity on the drift wall for the low and mean K_{th} cases (Figure 5.3.1.4.8-1c). The low K_{th} results in very low relative humidity in the early postclosure times: it starts at 3 to 5 percent from 50 to 60 years and gradually increases, up to 60 percent at 1,000 years. Relative humidity calculated for the mean value of K_{th} is 20 percent in the 50- to 60-year time frame, increasing to 60 percent by 400 years. The comparable, time-wise, values for the high K_{th} are 28 percent and 70 percent, as shown on Table 5.3.1.4.8-2.

However, the impact on performance due to the differences in relative humidity is more significant during later times, when humidity exceeds 60 percent. As noted in Table 5.3.1.4.8-2 the humidity reaches 60 percent for the mean K_{th} within 400 years after emplacement and increases to 95 percent at 1,000 years after emplacement. The relative humidity calculated for the high K_{th} case is 70 percent at 400 years (17 percent higher than the mean value results) and nearly 100 percent at 1,000 years. For the high K_{th} case, those same relative humidity levels of the mean K_{th} case would occur at 280 and 700 years, respectively. The time required for the drift wall to attain ambient (near 100 percent) relative humidity is 900, 1,000, and 2,000 years for the high, mean, and low K_{th} cases, respectively. If the K_{th} values were actually lower than the mean used in the performance assessment, the results would be bounding; the relative humidity would be significantly lower for longer periods of time.

The relative humidity results for the drip shield (Figure 5.3.1.4.8-1d) are sensitive to K_{th} for values of K_{th} smaller than the mean; however, they are relatively insensitive for values of K_{th} larger than the mean value used in the MSTH model analyses. The most divergent case, low K_{th}, has a much lower relative humidity than either the mean or high K_{th} case for the first 2,000 years. Beyond 2,000 years, there are minor differences between these cases.

Sensitivity of the MSTH model liquid saturation in the invert material was also evaluated. Figure 5.3.1.4.8-2 shows the predicted liquid saturation for the same locations as the temperature and relative humidity assessments discussed above. The results are for the upper invert layer directly below the drip shield in the central portion of the drift (Figure 5.3.2.3-1). These analyses were performed for the mean infiltration flux case. The liquid saturation in the invert is zero until about 2,100 years after emplacement for the mean and high K_{th} cases and about 3,200 years for the low K_{th} case. From the onset of rewetting (i.e., onset of nonzero liquid saturation values) until about 13,000 years after emplacement, the liquid saturation within the invert is somewhat sensitive to the K_{th} used in the model. The difference in liquid saturation at 4,000 years is only 2.6 percent between the high K_{th} case (2.8 percent saturation) and the low K_{th} case (0.2 percent saturation). There is approximately a 2,000-year difference in time for liquid saturation to reach 2 percent, which is nearly 3,000 years for the high K_{th} case and 5,000 years for the low K_{th} case. The high and mean K_{th} cases are quite similar. This leads to the conclusion that it is likely that only much lower K_{th} values would significantly change the liquid saturation conditions in the invert for K_{th} variations greater than those considered. In the long-term period of the HTOM, there is essentially no difference due to variation in K_{th}.

A set of analyses similar to those of the HTOM were performed for the LTOM. These analyses using the LDTH submodel considered the same range of thermal conductivity and the same location in the potential repository footprint as the HTOM analyses.

As can be observed in Figures 5.3.1.4.8-3a and 5.3.1.4.8-3b, temperatures on the drift wall and the drip shield were sensitive to the K_{th} used in the models for as long as 100,000 years. The MSTH model temperature results were more sensitive to variability in K_{th} values (represented by values lower than the mean) than they were to values above the mean. The drift wall peak temperatures for the low K_{th} values were approximately 88°C, compared to 73°C for the mean. The difference was 15°C, which was about 21 percent higher than the mean value temperatures. The difference between the mean and high K_{th} temperatures was much less, around 3°C, 70°C for the high K_{th} compared to 73°C for the mean value, which is only 4 percent lower than the temperatures for the mean value. At 10,000 years after emplacement, the difference between the mean and high K_{th} results is negligible, while there is a difference of 5°C between the low and mean K_{th} cases. For the high and mean value cases, the drift wall temperatures drop below 70°C at 1,400 years after emplacement, whereas the low K_{th} temperatures do not drop below 70°C until 3,800 years after emplacement.

A similar sensitivity trend to the K_{th} values used in the MSTH model analyses was observed in the temperatures on the drip shield. The peak temperature for the low K_{th} was 93°C, compared to 77°C for the mean and 75°C for the high K_{th} values. The differences between the mean calculation results and the low and high K_{th} calculation results are 21 percent and 3 percent, respectively. Again, the differences persist for up to 100,000 years, while the difference between the mean and high K_{th} results essentially become insignificant within about 10,000 years. The temperatures drop to below 70°C at approximately 2,000 years and 4,000 years for the mean/high and low K_{th} values, respectively.

There are no differences in calculated relative humidity on the drift wall for the low, high, and mean K_{th} cases (Figure 5.3.1.4.8-3c). All cases result in nearly 100 percent relative humidity for all times. The lower temperatures do not result in rock dryout, and the MSTH model analyses do not account for moisture removal by ventilation. Therefore, the relative humidity remains close to 100 percent (ambient conditions) for all times. The impact of ventilation is discussed in Section 5.3.2.4. The relative humidity results for the drip shield (Figure 5.3.1.4.8-3d) are very insensitive to the K_{th} used in the MSTH model analyses.

Figure 5.3.1.4.8-4 shows the predicted liquid saturation for the same locations as the temperature and relative humidity assessments discussed above. The results are for the upper invert layer directly below the drip shield in the central portion of the drift (Figure 5.3.2.3-1). These analyses were performed for the mean infiltration flux case. The liquid saturation in the invert is zero for all thermal conductivity cases until about 1,100 to 1,200 years after emplacement for the mean and high K_{th} cases and about 2,000 years for the low K_{th} case. From the onset of rewetting until 20,000 years after emplacement, there is a degree of sensitivity of liquid saturation within the invert to the K_{th} used in the model. The difference in liquid saturation at 7,000 years is 1.8 to 1.9 percent liquid saturation between the high K_{th} case (5.1 percent saturation) and the low K_{th} case (3.2 to 3.3 percent saturation). There is a 2,000-year difference in time when the invert liquid saturation reaches 3 percent between the high and low K_{th} cases, which reach 3 percent liquid saturation at 3,000 and 5,000 years respectively. The time difference increases up to 3,000 years for 3.2 percent between the high and low K_{th} cases.

Comparison of Results of Higher- and Lower-Temperature Operating Modes-Peak temperatures on the drift wall in the central portion of the potential repository for the HTOM and the LTOM are about 148 and 73°C, respectively, under mean infiltration and permeability conditions. The temperatures decrease to ambient (i.e., approximately 22.5°C) around 100,000 years. The relative humidity on the drift wall for the HTOM drops to about 20 percent about 60 years after emplacement, then increases to 95 percent at about 1,000 years. The temperatures at the time that the drift wall relative humidity approaches 100 percent are about 90°C, and decrease to 70°C around 4,000 years. Thus, there is a period of about 3,000 years when the relative humidity is nearly 100 percent and temperatures are higher than 70°C. For the LTOM, the relative humidity is always nearly 100 percent. The drift wall temperatures for the LTOM are between 70 and 74°C from about 400 to 1,500 years. Thus, there is a period of about 900 years when the temperatures are slightly above 70°C and the relative humidity is nearly 100 percent. For the LTOM, the drip-shield relative humidity is very insensitive to K_{th}. For the HTOM, drip-shield relative humidity is sensitive to K_{th} for values less than the mean K_{th}; this sensitivity lasts for about 2,000 years. For values of K_{th} greater than the mean value, relative humidity is much less sensitive, with relative humidity being somewhat higher for the high K_{th} case during the first 1,100 years.

Summary–The MSTH model results for the drift wall and drip shield are sensitive to the variations in K_{th} used as input in the models for the mean infiltration case up to as long as 100,000 years after emplacement. The MSTH model temperature results were more sensitive to variability in K_{th} values represented by values lower than the mean than they were to values above the mean. For the HTOM, the drift wall peak temperatures for the low K_{th} values were 70°C higher than for the mean case, nearly 220°C compared to 148°C for the mean, compared to a 8°C difference between the mean and high K_{th} temperatures (136°C). At 1,000 years after emplacement, the difference between the mean and high K_{th} results is negligible (2 to 3°C), with the mean K_{th} temperatures about 96° to 97°C, the boiling point of water. At 1,000 years after emplacement, the low K_{th} drift wall temperatures are 112°C, and rock at the drift wall would remain above the boiling point for approximately another 1,000 years.

For the LTOM, the drift wall peak temperatures for the low K_{th} values were approximately 88°C, compared to 73°C for the mean case. The difference between the low and mean cases, 15°C, is about 21 percent higher than the mean-value temperatures. The difference between the mean and high K_{th} temperatures was only 3°C, 70°C for the high K_{th}, compared to 73°C for the mean value, which is only 4 percent lower than the temperatures for the mean value. At 10,000 years after emplacement, the difference between the mean and high K_{th} results is negligible, but a 5°C difference between the low and mean cases remains. For the high and mean K_{th} cases, the drift wall temperatures drop below 70°C at 1,400 years after emplacement, whereas the low K_{th} temperatures do not drop below 70°C until 3,800 years after emplacement.

Drip shield temperatures exhibited similar sensitivity to the K_{th} values used in the MSTH model analyses. These sensitivities persist for up to 100,000 years. For the HTOM, the peak drip shield temperature of the low K_{th} was 234°C, compared to 160°C for the mean and 150°C for the high K_{th} values. The difference between the mean and high K_{th} results essentially becomes insignificant within about 1,000 years. The temperatures drop to the boiling point of water at about the same time as the drift wall temperatures, approximately 1,500 and 2,000 years for the mean/high and low K_{th} values, respectively. For the LTOM, the peak temperature for the low K_{th} was 93°C, compared to 77°C for the mean and 75°C for the high K_{th} values. The differences between the mean calculation results and the low and high K_{th} calculation results are 21 percent and 3 percent, respectively. The difference between the mean and high K_{th} results essentially becomes insignificant within about 10,000 years. The temperatures drop to below 70°C at approximately 2,000 and 4,000 years for the mean/high and low K_{th} values, respectively.

Only during the first 13,000 years after emplacement in the HTOM and 20,000 years after emplacement in the LTOM, respectively, is the saturation in the invert material somewhat sensitive to the values of K_{th} used in the MSTH model. For the HTOM, the liquid saturation in the invert is zero for all the thermal conductivity cases until about 2,100 years after emplacement for the mean and high K_{th} cases and about 3,200 years for the low K_{th} case. After the onset of saturation until about 13,000 years after emplacement, the saturation at 4,000 years is only 2.6 percent between the high K_{th} case (2.8 percent saturation) and the low K_{th} case (0.2 percent saturation). Thus, although there is sensitivity with saturation of less than 5 percent, the implications on performance are minimal. It is likely that only much lower K_{th} values would significantly change the saturation conditions in the invert for thermal conductivity variations greater than those considered. In the long-term period of the HTOM, there is essentially no difference due to variation in K_{th}. For the LTOM, the liquid saturation in the invert is zero for all the thermal conductivity cases until about 1,100 to 1,200 years after emplacement for the mean and high K_{th} cases and about 2,000 years for the low K_{th} case. There is a difference in saturation of 1.8 to 1.9 percent between the high K_{th} case (5.1 percent saturation) and the low K_{th} case (3.2 to 3.3 percent saturation) at 7,000 years. There is a 2,000-year difference in time between the high and low K_{th} cases, when the invert saturation reaches 3 percent, which reach 3 percent saturation at 3,000 and 5,000 years, respectively. The time difference increases up to 3,000 years for 3.2 percent between the high and low K_{th} cases.

5.3.1.4.9 Sensitivity of Multiscale Thermal-Hydrologic Model Results to Lithophysal Porosity

Sensitivity analyses of the impact of K_{th} uncertainties, largely due to lithophysal porosity impacts on thermal conductivity, were discussed in Section 5.3.1.4.8. In addition to the impacts on the thermal conductivity, the lithophysal porosity can also impact the heat capacity. Heat capacity is a function of rock mass density, and therefore subsequently a function of porosity. The heat capacity, thus, will decrease with increased porosity. Mapping data along the ECRB drift walls (Mongano et al. 1999 [DIRS 149850]) indicate that the mean lithophysal porosity of the lower lithophysal unit is 0.125 (see Section 4.3.5.3.2). The matrix porosity of the lower lithophysal unit (tsw35) is 0.115 (DTN: MO9901RIB00044.000 [DIRS 109966]). Because the lithophysal porosity is roughly equal to the matrix porosity, uncertainty in the lithophysal porosity can significantly impact the porosity and the heat capacity used in the MSTH model analyses.

Sensitivity studies were performed using the LDTH submodel of the *Multiscale Thermohydrologic Model* (CRWMS M&O 2000 [DIRS 149862]) to consider the effects of uncertainties in the lithophysal porosity on both thermal conductivity and heat capacity (BSC 2001 [DIRS 155008]), which in turn affect temperature, relative humidity, and liquid saturation at the drift wall and drip shield (Buscheck 2001 [DIRS 155243]). These sensitivity studies were performed for the same potential repository location as sensitivity studies in Section 5.3.1.4.8, which considered the lithophysal porosity on thermal conductivity alone. By comparing the results of the mean, high, and low lithophysal porosity results with the K_{th} analyses (Section 5.3.1.4.8), an assessment can be made of the sensitivity of the results to the lithophysal porosity, or more specifically to the influence of lithophysal porosity on heat capacity. Figure 5.3.1.4.9-1 shows the first analysis, which considered the effects that the range of lithophysal porosity (Table 5.3.1.4.9-1) had on the temperature and relative humidity on the drift wall and drip shield for a location in the center of the potential repository (location L5C3 reference) for the HTOM with the mean infiltration flux. Although the analyses were for the L5C3 location, they are applicable to the portion of the potential repository in which the host rock is the Tptpll unit, which comprises more than three-quarters of the potential repository area.

As can be observed by comparing the results shown on Figure 5.3.1.4.8-1a with the results shown on Figure 5.3.1.4.9-1a, the peak temperatures on the drift wall were 2 to 3°C cooler for the low lithophysal porosity case that included effects of the porosity on the heat capacity than that which did not. Likewise, peak temperatures were 16°C higher for the high lithophysal porosity than for the comparable case from Section 5.3.1.4.8 that did not include these effects on the heat capacity. Similar, but of smaller magnitude, differences were noted for the temperatures on the drip shield (Figures 5.3.1.4.8-1b and 5.3.1.4.9-1b). The differences for the drift wall and drip shield disappeared within 1,000 years of emplacement. Relative humidity differences were noted for the drift wall only, and only for the low lithophysal porosity case where there was an approximately 3 percent relative humidity difference when the porosity impacts on the heat capacity were considered (Figures 5.3.1.4.9-1c and 5.3.1.4.8-1c). There was no impact on the drip shield relative humidity (Figures 5.3.1.4.9-1d and 5.3.1.4.8-1d). Invert saturation (Figure 5.3.1.4.9-2) was not affected by neglecting the influence of lithophysal porosity on heat capacity. These observations indicate that neglecting the influence of lithophysal porosity on heat capacity will not add to uncertainty in the results from the MSTH model.

Comparisons of results for the LTOM with and without consideration of the influence of lithophysal porosity on heat capacity reveal no difference. This is seen by comparing results of the analyses of temperatures on the drift wall and drip shield that included consideration of the effects of lithophysal porosity on heat capacity (Figures 5.3.1.4.9-3a and 5.3.1.4.9-3b) with the results of the analyses that did not include the influence of lithophysal porosity on heat capacity

(Figures 5.3.1.4.8-3a and 5.3.1.4.8-3b). There is no difference in any of the curves. This result is consistent with the conclusions for the HTOM.

Figure 5.3.1.4.9-4 shows the predicted liquid saturation for the same location as the temperature and relative humidity assessments discussed above. The results are for the upper invert layer that is directly below the drip shield in the central portion of the drift (Figure 5.3.2.3-1). These analyses were performed for the mean infiltration-flux case. Comparison of Figure 5.3.1.4.9-4, which shows the results of analyses that considered the influence of lithophysal porosity on heat capacity, with Figure 5.3.1.4.8-4, which does not include the consideration of the influence of lithophysal porosity on heat capacity, indicates that there is no impact on the MSTH model invert saturation results as a result of neglecting the influence of lithophysal porosity on heat capacity.

5.3.1.4.10 Sensitivity to Invert Thermal Conductivity

The current design for the invert consists of a set of carbon steel beams crossing the drift and anchored to the drift wall. The beams are stabilized by longitudinal connectors and crushed tuff gravel ballast. The steel contacts the lower drift wall at the edges of the invert, and the lower portion of the drift wall contacts only the ballast. The carbon steel (as-built) has a higher thermal conductivity than the crushed tuff ballast. However, the carbon steel corrodes in a few hundred to a few thousand years, and the conductivity of the resulting iron oxide fragments is more similar to the ballast than to steel. Therefore, during much of the thermal period, the conductivity of the invert will be lower than its initial value.

The uncertainty (and temporal variability) of the invert thermal conductivity is exacerbated by the geometry of the steel structure. In regions that include both ballast and portions of beams, the invert will have a higher lateral or axial thermal conductivity than vertical conductivity. The software used in the MSTH model currently does not have the capability to input anisotropic thermal conductivity for different regions. This capability could be added, or the effect could be mitigated by a careful choice of invert layer geometry. The effect of the beam structure has been evaluated in a conduction-dominated regime by using the ANSYS software, which does have anisotropic conductivity (CRWMS M&O 2000 [DIRS 142736]). In this section, the invert thermal conductivity is varied parametrically to determine its influence on in-drift temperature distribution.

The LDTH submodel (CRWMS M&O 2000 [DIRS 149862]) was used in the sensitivity analysis (Reed 2001 [DIRS 155076]). The submodel results are suitable for determining the sensitivity of TH parameters to invert thermal conductivity. However, these sensitivity results do not include edge effects, variability of infiltration across the potential repository footprint, or three-dimensional in-drift phenomena. The MSTH model results for the HTOM described in Section 5.4 should be used if values of TH parameters are needed, rather than the sensitivity of those parameters to uncertainty of invert thermal conductivity.

The two-dimensional LDTH submodel was implemented for the L5C3 location in the potential repository footprint (as in a number of other sensitivity evaluations). This location has a thick cover of lower lithophysal rock that is not near the interface with the middle non-lithophysal subunit above. The surface infiltration rates (based on the methodology and input data in CRWMS M&O (2000 [DIRS 149862]) at this location are 5.7 mm/yr for the present-day climate

(0 to 600 years), 15.1 mm/yr for the monsoonal climate (600 to 2,000 years), and 23.2 mm/yr for the glacial-transition climate (beyond 2,000 years). The submodel included explicit thermal radiation between the drip shield and drift wall, and it applied a correlation-based effective thermal conductivity approach for natural convection heat transfer. Mass transfer within the emplacement drift was computed using a bulk permeability of 10^{-8} m^2 for the in-drift air elements (Buscheck 2001 [DIRS 155243]), which was a compromise between adequate mass transfer and computer run time (see Section 5.3.2.4.5). The heat source in the model was volumetrically averaged within the volume enclosed by the drip shield. The calculations used the same initial linear heat loading, 1.3534 kW/m, as the HTOM, and they also used the same ventilation parameters: 50 years of forced ventilation at an assumed heat removal efficiency of 70 percent.

The invert geometry in the calculation includes two vertical layers (regions), with two gridblocks in the lower layer and four gridblocks in the upper area (Figure 5.3.2.3-1). The sensitivity study considered a range of material thermal conductivity for the upper invert layer. The lower invert material thermal conductivity was 0.15 W/m•K for all the sensitivity runs because it included only ballast without the steel beams.

Table 5.3.1.4.10-1 shows the range of invert thermal conductivity used in the study. The base case thermal conductivity was the lowest value considered; it was based on the decrease of the as-built value toward that of crushed tuff as the carbon steel corrodes. Additionally, low thermal conductivity in the invert was expected to increase the in-drift temperatures because overall heat transfer would be somewhat less effective. The as-built case assumed that the steel does not corrode. The additional-steel case assumed that the amount of steel in the invert design is increased at some future date. Two overlapping continua were used in the model, for compatibility with the dual continuum approach in the host rock. Because a realistic, dual-continuum, hydrologic property set for crushed tuff is not yet available, the continua had identical thermal and hydrologic properties for the base, as-built, and additional-steel cases, with the thermal conductivity equally split between the two continua. A fourth case, designated the intermediate case, used a steel-like conductivity in one continuum and a ballast-like conductivity in the other.

Five locations in the engineered barrier system (EBS) were used to evaluate the sensitivity to the invert thermal conductivity, using material-appropriate TH parameters. The five locations and associated parameters included:

- The top of the drip shield (temperature and relative humidity)
- The base of the drip shield (temperature and relative humidity)
- The crown of the drift wall (temperature and liquid saturation)
- The rib (i.e., the widest point, sometimes referred to as the springline) of the drift wall (temperature and liquid saturation)
- The center of the lower level of the invert (temperature and liquid saturation).

These five EBS locations were selected to illustrate the potential for vertical and horizontal variability with the drift to be influenced by the invert thermal conductivity.

Figures 5.3.1.4.10-1 and 5.3.1.4.10-2 illustrate the temperature-time histories at two of the five selected EBS locations. The temperature histories at the other three locations (drift wall rib, drip shield top, and drip shield base) were similar to the drift wall crown, both in terms of general shape and the tight spacing (insensitivity) of the four thermal conductivity cases. Table 5.3.1.4.10-2 shows the peak temperatures at all five locations. The calculated time of peak temperature for the HTOM was calculated to occur between 65 and 70 years after emplacement (15 to 20 years after closure). The largest temperature variation was in the lower invert, which can vary by about 9°C over the range of conductivity investigated. The other four locations had peak temperature variation between conductivity cases of 9°C or less. Figure 5.3.1.4.10-1 and Table 5.3.1.4.10-2 indicate that the drift wall and drip shield temperatures are slightly higher for the base (low) invert thermal conductivity case than for the higher thermal conductivity cases. For the lower conductivity case, the rate of conduction heat transfer downward through the invert was reduced, which elevated temperatures on the invert floor and at the base of the drip shield. The hotter floor surface exchanged energy with the top and side of the drift (crown and rib) by radiation, thus elevating temperatures there as well. In the lower half of the invert, Figure 5.3.1.4.10-2 illustrates that a reduction in the heat transfer rate through the upper portion of invert, as expected for the base (low) invert conductivity cases, caused somewhat lower temperatures in the lower region of the invert material. The lower invert temperature was also more sensitive to thermal conductivity than the other locations in the drift. The lowest upper invert thermal conductivity (0.15 W/m•K) caused the largest temperature drop across the invert.

The liquid saturation in the drift wall and lower portion of the invert are shown in Figures 5.3.1.4.10-3 and 5.3.1.4.10-4 (the drift wall rib saturation histories are similar to those shown for the crown). For all the invert conductivity cases, the host rock (drift wall) matrix saturation falls quickly and does not resaturate until about 1,000 years. At this time, rock temperature drops to the local saturation temperature and water quickly returns to the host rock. Figure 5.3.1.4.10-4 indicates that the invert liquid saturation history is more sensitive to the invert conductivity than is the host rock saturation. The base thermal conductivity case (0.15 W/m•K) shows the invert saturation becoming nonzero at about 1,300 years, increasing to a maximum value of about 0.1, then dropping to a long-term value of 0.057. A rapid transition through the boiling point (Figure 5.3.1.4.10-2) for this case results in rapid rewetting at this location. The other three cases show nonzero invert saturation at about 2,200 years, with maximum saturation of about 0.057. All the cases converge to the same long-term value (0.057), as expected, when the temperature returns to ambient. The period of high invert saturation for the low-conductivity case and the oscillations during rewetting for the lowest two conductivity cases have not been explained. The simple treatment of hydrologic properties in the invert (compared to the host rock) is a potential cause that is being evaluated in support of a potential license application.

Figure 5.3.1.4.10-5 shows the relative humidity at the drip shield top (the drip shield base is similar). The relative humidities are similar over the range of invert thermal conductivity investigated. The base-case thermal conductivity (0.15 W/m•K) resulted in slightly lower relative humidity at the drip shield due to slightly higher temperatures (Table 5.3.1.4.10-2).

Summary–The three higher invert thermal conductivity cases produce similar temperature, liquid saturation, and relative humidity at the five EBS locations considered. The base case (0.15 W/m•K) invert thermal conductivity case resulted in differences in all three TH parameters. The late time values for all cases are similar after about 100,000 years. The invert saturation for the base case invert conductivity has an earlier rewetting initiation and a lengthy (100,000 years) higher-saturation plateau prior to converging on the same long-term saturation as the other cases. The values of temperature for the intermediate case are within a few degrees of the base case, allowing other sensitivity calculations in Section 5 to use either of the invert conductivity values.

5.3.1.4.11 Sensitivity to Design and Operational Parameters

The analyses presented in this report focus on three goals: incorporating new science, quantifying uncertainties, and evaluating the performance and uncertainty associated with HTOM and LTOM. This section discusses the sensitivity of TH parameters to design and operating parameters that could be used to achieve a LTOM goal.

Figure 5.3.1.4.11-1 depicts the HTOM and LTOM in terms of values of peak waste package temperature resulting from different choices of design and operating parameters. The figure shows that the HTOM has waste package peak temperatures of about 175°C, lower than the peak values presented in the *Viability Assessment of a Repository at Yucca Mountain, Total System Performance Assessment* (DOE 1998 [DIRS 100550], Volume 3, Figure 3-22), which shows a peak temperature of about 200°C using bin-averaged, rather than hottest waste package, temperatures. Two LTOM options are shown, both resulting in peak waste package temperatures of about 85°C based on two-dimensional calculations.

Three design parameters—drift diameter, drift spacing, and waste package capacity—are shown in the inner portion of Figure 5.3.1.4.11-1. These parameters were held constant for the purposes of this report, which focuses on determining performance and associated uncertainty for a range of thermal operating environments. If the site is recommended, design parameters can be varied during the preparation of a license application to optimize a combination of criteria, including worker safety, cost, and reduction in performance uncertainty.

The outer portion of Figure 5.3.1.4.11-1 shows operating parameters, including waste package spacing, forced and natural ventilation rates, and ventilation duration. These parameters can be changed even after a repository has been constructed. The two LTOM options use different values of operational parameters to approach the same TH conditions. The option analyzed in this document uses the first 64 drifts in the footprint (a contiguous, planar area), variable gaps between waste packages (1.1-m average), and 300 years of forced ventilation at a rate of 15 m^3/s. The resulting linear heat loading at emplacement of this option is 1.3534 kW/m (Buscheck 2001 [DIRS 155243]).

Another lower-temperature option uses a larger footprint, has wider gaps between waste packages (2-m average), and shifts from forced to natural ventilation after 50 years (BSC 2001 [DIRS 155010]; BSC 2001 [DIRS 155011]). The natural ventilation rate used in the second reference is an average of 3 m^3/s for the 50- to 100-year period and 1.5 m^3/s for the 100- to 300-year period. The resulting linear heat loading at emplacement of this option is 1.0 kW/m.

The two options trade forced ventilation duration and waste package spacing (and potential repository footprint).

Natural ventilation and other methods to achieve lower potential repository temperatures have been the subject of study for several years (BSC 2001 [DIRS 154855]; CRWMS M&O 2000 [DIRS 152269]; CRWMS M&O 2000 [DIRS 152146]). The lower-temperature option shown in (Figure 5.3.1.4.11-1) is based on design and operational parameters developed from sensitivity calculations in these three references. Additional documentation is in BSC (2001 [DIRS 155010]) and BSC (2001 [DIRS 155011]).

The in-drift TH parameter histories, including variability across the potential repository footprint, are shown in Section 5.4.2 for the LTOM. The MSTH model calculations (Buscheck 2001 [DIRS 155243]) were repeated for the same AML and linear heat loading of 1.13 kW/m as the LTOM base case (see Table 5.1-1). The new calculation (Buscheck 2001 [DIRS 155243]) used a line loading arrangement with 10-cm gaps between all waste packages, rather than more widely spaced waste packages. The linear heat loading was maintained at the same level, since the waste packages were moved together by de-rating the hotter waste packages. The de-rating was done simplistically, by removing spent nuclear fuel assemblies from the hotter PWR waste packages until the target heat loading was achieved (at the 16 fuel assembly level). If a lower-capacity waste package option is developed during a potential license application, it could achieve goals of lower peak power by using smaller PWR waste packages or by blending BWR and PWR assemblies in the same waste package. Flexibility could be reserved for the blending of the two types of assemblies by developing an adapter-insert that would fit into the PWR basket slot and contain an opening the size of the smaller BWR assemblies.

Figure 5.3.1.4.11-2 compares the postclosure distribution of peak waste package temperature and relative humidity across the potential repository footprint for the LTOM option described in this report and the de-rated waste package capacity option for the medium infiltration history case, although the MSTH model results also include cases for lower and higher infiltration levels. The distributions are displayed as cumulative complementary distribution functions; the values on the y-axis are the fraction of waste packages hotter than the indicated value on the x-axis. The base case resulted in 62 percent of the waste packages not exceeding the goal of 85°C, and a peak of 91.2°C for the hottest waste package in the 6,710 calculated waste package temperature-time histories. The abstracted temperature histories used in TSPA are somewhat lower because histories are grouped into bins, within which the average is used. The de-rated waste package case resulted in 74 percent of the waste packages not exceeding the goal of 85°C, and a peak of 87.9°C for the hottest waste package. The de-rated waste package option had slightly cooler results for the same potential repository footprint. The cooler temperatures are due to the smaller range of thermal powers among the waste packages and the more effective radiation heat transfer between closely spaced waste packages.

For waste packages that exceed the 85°C goal, a low humidity can prevent the formation of aqueous films that are required for corrosion initiation. Figure 5.3.1.4.11-2 also shows the postclosure relative humidity distribution (among the 38 percent of the ensemble of waste packages that exceed 85°C for some period of time in the LTOM base case) when the temperature of each waste package falls below 85°C. The initiation threshold for crevice corrosion of 85°C is based on more aggressive water chemistry than is expected on waste package surfaces (Section 6).

To compare other options, a simplified version of the MSTH model was used (Buscheck 2001 [DIRS 155243]). In the simpler model, the same four submodels were used, but only a single location (L5C3) was used for the smeared-heat-source drift-scale temperature (SDT) and line-source drift-scale thermal-hydrologic submodels. The L5C3 location is near the potential repository center and is within the lower-lithophysal stratigraphic unit.

Figure 5.3.1.4.11-3 shows postclosure temperature and relative humidity histories (Buscheck 2001 [DIRS 155243]) for the hottest waste package surface for three LTOM implementations that share the same areal mass loading of 45.7 MTU/acre: the LTOM base case, the de-rated waste package case, and a wider drift spacing case that uses the HTOM waste package arrangement, but with a drift spacing of 97 m instead of 81 m. As summarized in Table 5.3.1.4.11-1, the peak temperatures are 90.0°C for the base case, 87.3°C for the de-rated waste package case, and 88.8°C for the wider drift spacing case. These results indicate that all three methods achieve similar temperatures for LTOM designs. Line loading with a limited range of waste package thermal powers is most effective at limiting peak temperature, and wider spacing of line-loaded drifts is more effective than spacing waste packages within the drifts. The relative effectiveness of these design and operating parameters (waste package capacity, drift spacing, and waste package spacing) is consistent with the conceptual understanding of three-dimensional radiation heat transfer among the waste packages.

A comparison of Figures 5.3.1.4.11-2 and 5.3.1.4.11-3 shows that the simplified MSTH model calculates peak temperatures about 1°C less than the full MSTH model. It was expected that the peak temperatures would be somewhat lower because it is not likely that the location chosen for the simplified MSTH model would be the location of peak power. The location was chosen, however, to be in a central region with low infiltration flux so that it would be near the overall peak temperature. The advantage of using the simplified MSTH model is that additional design variables can be investigated with a smaller suite of calculations, yet with results (at the chosen location) that are the same as the full MSTH model results.

The postclosure relative humidity histories at the hottest waste package surface are shown in Figure 5.3.1.4.11-3 for the three LTOM cases. Depending on the composition of the dust on the waste package surface, the threshold relative humidity for water film formation (deliquescence) varies. Figure 5.3.1.4.11-3 can be used to determine the time at which the threshold humidity is reached. This value can then be used with the temperature panel of the same figure to estimate the likelihood of crevice corrosion during the thermal pulse for the hottest waste packages in the potential repository. The figures show that, during the time that the surfaces of some waste packages are above 85°C, the humidity ranges between 37 and 61 percent for the LTOM base case, between 48 and 69 percent for the wider drift spacing case, and between 43 and 60 percent for the de-rated waste package case. The duration in which temperatures are above 85°C is about 500 years for all three cases.

Summary–Design and operating parameters can be used to achieve LTOM goals. The initial calculations for three different lower-temperature options predicted temperatures within 5°C of the 85°C goal. A slightly modified operating mode could achieve the goal. Use of operating parameters to maintain temperature flexibility offers the advantage of preserving some flexibility even after construction of a potential repository. A simplified MSTH model can be used to calculate local temperatures while maintaining the fidelity of the calculations to the potential repository footprint, the infiltration flux map, and waste package spacing and power distribution. The simplified model runs faster and produces temperatures within about 1°C of the full MSTH model. For the 300-year forced ventilation option, waste package peak temperature can be limited to about 85°C by adjusting waste package capacity, drift spacing, or waste package spacing. Adjusting waste package capacity was the most effective of the three methods because of the smaller range of waste package thermal powers. Adjusting waste package spacing was the least effective because of the reduced effectiveness of radiative smoothing of the in-drift thermal power distribution. However, the differences in effectiveness only resulted in a peak waste package temperature variation of about 3°C among the three cases investigated.

5.3.2 Ventilation and Convection Modeling of In-Drift Thermal-Hydrologic Conditions

This section discusses phenomena involving movement of gas and transfer of heat within emplacement drifts. There are four such phenomena, which are discussed conceptually below.

Two-Dimensional Convection–Air moves naturally within a plane perpendicular to the drift axis, driven by the temperature gradient between the warmer waste package and the intermediate-temperature drip shield, and also between the drip shield and cooler drift wall (Figure 5.3.2-1 illustrates the air flow pattern). The figure shows the flow pattern in a quarter-scale test (Jurani 2001 [DIRS 155128]) in an insulated pipe without a drip shield. For the flow pattern beneath the drip shield in a potential repository following closure, the air rises above the waste package, turns outward and falls along the inner surface of the drip shield, transferring heat to the drip shield as it moves. The cooler air at the bottom of the drip shield rises along the waste package, picking up more heat. A similar flow pattern would be established between the drip shield and drift wall. These flow patterns augment the heat transfer due to thermal radiation between the components. Natural convection is more important during the postclosure period when high-flow-rate forced ventilation is absent.

Natural convection is driven by the temperature difference between the hot drip shield and cooler drift wall. Radiative heat transfer is driven by the difference between the fourth power of those temperatures; therefore, thermal radiation is most important at higher temperatures. For the LTOM, thermal radiation is less effective than for the HTOM, and two-dimensional convection of air can be an important contributor to limiting the temperature of the waste package.

Three-Dimensional Convection–Air moves within segments of the emplacement drift. This convection is produced by the temperature gradient along the drift axis, and the flow patterns are three-dimensional, as illustrated conceptually in Figure 5.3.2-2. There is axial flow from hotter to cooler regions under the crown of the drip shield and under the crown of the emplacement drifts. Cooler air returns in the opposite direction near the invert. There are two scales of this convection. The smaller scale is between a group of waste packages that have different thermal powers due to their differing waste contents. The larger scale is between the sections of the emplacement drifts near and far from the edge of the potential repository. The edge regions are cooler because, in addition to the heat flow upward and downward from the potential repository horizon, the edge regions also have lateral heat transfer outward from the perimeter drifts. This phenomenon is most important in the postclosure period when high-flow-rate forced ventilation is absent.

Natural Circulation Within the System of Drifts and Natural Ventilation to the Surface–After closure, when forced ventilation ceases, air continues to move within the system of underground drifts, although at reduced rates and possibly in different flow patterns than described above. When this flow includes a path to the surface (through fractures or intentionally open shafts), it is termed "natural ventilation." The difference in air density at the entrance and exit of the loop drives natural ventilation. Heat produced by the waste packages contributes to this natural ventilation.

When air flow is confined to a closed path within the natural fractures and the underground system of drifts, it is termed "natural circulation." Heat from the waste packages drives natural circulation. For natural circulation and natural ventilation, the transfer of heat from the emplacement drifts to the perimeter of the potential repository or the mountain surface, due to heating of the air in the emplacement drifts, is augmented by evaporation of water from near-field rock into the air. The movement of water and heat in this manner is important in that it can limit the temperature of the waste package and the seepage of liquid water into the emplacement drifts.

Forced Ventilation–During the preclosure period, fans will force air through the emplacement drifts, transporting heat and water. This ventilation will dominate the above three phenomena during the preclosure period and will remove a large fraction of the heat from the waste packages. Because the intensity of the heat source decreases with time as radionuclides decay, using a longer period of ventilation will reduce the peak temperatures that occur after ventilation ceases. Thus, extended ventilation is one option for attaining a LTOM.

The remainder of Section 5.3.2 discusses the goal of the in-drift gas movement models, the treatment in TSPA-SR (CRWMS M&O 2000 [DIRS 153246]), the improvements made to the TSPA modeling for the SSPA, and six sensitivity analyses at the process-model level. These sensitivity analyses are an independent line of work from the TSPA model because of the reduced extent of simplification and abstraction and because subsystem parameters are used (rather than dose rate) to develop insights.

5.3.2.1 Goal of the Models

Process models for in-drift convection and ventilation have improved significantly during the last few years. This subsection describes the goals for these models, in support of a potential license application. The following subsections describe the representation of convection and ventilation in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246], Section 3.3; CRWMS M&O 2000 [DIRS 149862], Section 6.6.1), recent improvements in support of uncertainty quantification for the Supplemental Science and Performance Analyses (SSPA), and application of those improved models for HTOM and LTOM.

For two-dimensional convection, the goal of the process model is to include a realistic representation of heat transfer within the drift in the MSTH model described in Sections 5.2 and 5.3.1. The process model should include evaporation and condensation due to differences, within the plane perpendicular to the drift axis, between the local air temperature and the temperatures of the waste package, drip shield, and drift wall. The fraction of the heat transferred to the rock by two-dimensional convection will increase with time, due to the less effective radiative heat transfer as temperature decreases. Similarly, accurate treatment of two-dimensional convection will be important for the LTOM.

For three-dimensional convection, the goal of the model is to include a realistic representation of heat transfer within the drift in the MSTH model described in Sections 5.2 and 5.3.1. The model should include local evaporation and condensation due to differences, along the drift axis, between the local air temperature and the temperatures of the waste package, drip shield, and drift wall. The significance of three-dimensional convection will vary with time. At times soon after closure, small-scale axial convection due to waste package power variability will be most important. Later, the cooling effect of the edge of the potential repository will drive larger-scale axial convection.

For natural circulation within the system of drifts and natural ventilation to the surface, the goal of the model is to include their influence on postclosure in-drift thermal-hydrologic conditions and to calculate the volume and paths of the post-closure air flow. These calculations should include the influence of evaporation and condensation of water on local air temperature and density. Results of the modeling can also be used by the design organization to determine if connecting drifts should be added to link the network of exhaust drifts with the perimeter drifts just prior to closure.

For forced ventilation, the goal of the model is to calculate the time-dependent efficiency of heat and water removal by ventilation, including the effects of evaporation and condensation of water. These results should be coupled to the MSTH model (Sections 5.2 and 5.3.1).

5.3.2.2 Representation in Total System Performance Assessment-Site Recommendation

For two-dimensional convection, the LDTH submodel of the MSTH model (CRWMS M&O 2000 [DIRS 149862], Section 4.1.10; see also Section 5.2), used time-dependent equivalent heat transfer coefficients for the in-drift regions under and outside the drip shield TSPA-SR (CRWMS M&O 2000 [DIRS 153246], Section 3.3). These coefficients, which change with time due to the temperature effects on natural convection and radiative heat transfer, are based on concentric cylinder representations of the waste package, drip shield (after closure), and the drift wall. The radiation portion of the heat transfer coefficient was based on an analytic solution published by Incropera and DeWitt (1985 [DIRS 100623], p. 609, Equation 13.25). The two-dimensional convection portion of the heat transfer coefficient was based on an empirical correlation for concentric cylinders described by Kuehn and Goldstein (1978 [DIRS 130084]). The calculation of the equivalent heat transfer coefficient that includes convection and radiation is described in *Effective Thermal Conductivity for Drift-Scale Models Used in TSPA-SR* (CRWMS M&O 2001 [DIRS 153410]). The two-dimensional convection calculation was approximate because spatially-uniform coefficients were used within each air region, which is not consistent with the below-drift-center location of the waste package, and also does not consider the local air flow patterns.

Although the MSTH calculation includes vaporization of water from the near field rock into the drift air, it only accounts for a small fraction of the water that evaporates into the drifts from the rock. This limitation is the result of not including movement of air axially along the drift, which continually provides a dry-air moisture sink in the drift, into which water can vaporize.

For three-dimensional convection, the MSTH model described in Sections 5.2 and 5.3.1 calculates the influence of the edge of the potential repository and the spatial distribution of water infiltration on the temperatures along the drift axis. The model did not include the influence of these axial temperature variations on three-dimensional convection (of heat and water vapor) within segments of the emplacement drifts.

Natural circulation within the system of drifts and natural ventilation to the surface after closure were not included in the initial model of the HTOM.

For forced ventilation, a dry air flow model was coupled to a conduction (in the rock) thermal model to develop an initial estimate of ventilation efficiency (the ratio of the heat removed in the air to the heat released from the waste) for the HTOM. The result of this calculation was an efficiency of 74 percent for 50 years of ventilation at 15 m^3/s, as described in *Ventilation Model* (CRWMS M&O 2000 [DIRS 120903], p. 39). Quarter-scale tests (Jurani 2001 [DIRS 155128]) verified that the ventilation efficiency is greater than the calculated value for the HTOM (see Section 5.3.2.4.1). The model and tests did not include the effects of water evaporating from the rock into the air, which would increase the efficiency. A slightly conservative value of preclosure ventilation efficiency, 70 percent, was used in the multiscale thermal-hydrologic model. This was implemented by using only 30 percent of the thermal power of the waste packages for calculation of combined radiative and natural convection heat transfer from the waste packages to the drift wall during the preclosure period.

5.3.2.3 Reduction in Total System Performance Assessment Uncertainty Due to Model Improvements

For modeling of heat and mass transfer across the air gap in the drift, two aspects of the MSTH model were improved in support of the Volume 2 (McNeish 2001 [DIRS 155023]) TSPA. Both of these improvements resulted in higher confidence in calculated temperature histories of the drip shield and waste package. The specific improvements are discussed below.

Explicit Calculation of Thermal Radiation between the Drip Shield and Drift Wall in the Line-Source Drift-Scale Thermal-Hydrologic Submodel–In the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]), the heat transfer between the drip shield and drift wall was calculated using an equivalent heat transfer coefficient that accounted for thermal radiation and natural convection. Both the radiation and the natural convection correlations were based on concentric cylinders, and both correlations were evaluated using temperature time histories developed for prior designs.

The LDTH calculations in support of the HTOM and LTOM base-case TSPA calculations for the SSPA used explicit treatment of radiation between the drip shield and drift wall. Therefore, the use of an effective thermal conductivity (to decrease computational burden) was limited to the smaller heat transfer contribution of natural convection. This improvement removed part of the uncertainty due to approximate treatment of thermal radiation in prior TSPA calculations. These uncertainties were due to the geometric simplification associated with the concentric cylinder (without invert) correlation that was used. These uncertainties were also due, in part, to the evaluation of the correlation at temperature time histories that were not calculated specifically for the most current design.

Mass Balance in the Invert for the Line-Source Drift-Scale Thermal-Hydrologic Submodel–In checking the initial MSTH calculations for the SSPA Volume 2 (McNeish 2001 [DIRS 155023]) base cases, it was determined that a numerical instability was causing unphysical results to occur at some invert locations, usually near the side of the invert, and at some times, usually many thousands of years after closure. These results include oscillation of invert saturation and also include high fluxes into invert regions without corresponding increases in saturation or fluxes leaving these regions.

Two potential causes were identified for the numerical instability. The first was the equivalent continuum treatment of the invert gravel. Although the model calculates the hydrologic processes in the invert using two continua, there is a lack of continuum-specific hydrologic properties for the gravel rocks and the spaces between the rocks. Thus, the model is usually run with both continua having identical properties. The hydrologic treatment of the invert is being improved in support of a potential license application.

The second potential cause for the numerical instability was a fairly coarse gridding (Figure 5.3.2.3-1) combined with a large mismatch in thermal conductivity across small distances, due to the presence of the high-conductivity steel beams in the upper regions of the invert. In considering this situation, it was recognized that the carbon steel beams would corrode after several centuries of exposure to high-relative, humid air. After corrosion, the conductivity of the oxidized steel would be more similar to the conductivity of tuff gravel than to the original steel. Thus, the thermal conductivity of the invert was set to 0.15 W/m•K for all invert zones for the SSPA Volume 2 (McNeish 2001 [DIRS 155023]) base-case calculations. The result of this change was a significant decrease in the numerical instabilities observed in the invert saturation (Section 5.3.1.4.10 shows specific results).

The uncertainties associated with invert thermal properties and invert hydrologic treatment are important to different results of the model and different times. Prior calculations used a high thermal conductivity in the upper part of the invert (as-built conditions) for the entire calculation period. After the steel degrades, this assumption would result in higher calculated heat flow through the invert and lower calculated in-drift temperatures, compared to the expected situation. The underprediction of in-drift temperatures would be manifested beginning a few decades to centuries after humidity increases in the drift. Thus, the underprediction of in-drift temperatures could affect peak temperature calculations for the LTOM. The current calculations use a degraded thermal conductivity for the invert steel for the entire calculation period. Until the steel degrades, this assumption would result in lower calculated heat flow through the invert and higher calculated in-drift temperatures, compared to the expected situation. For the HTOM, high humidity conditions are precluded in the drift for centuries to about 1,000 years after closure, depending on the location with respect to the potential repository edge and the value of humidity at which carbon steel begins to corrode. Since the HTOM peak in-drift temperatures occur within a few decades of closure, the treatment of invert conductivity in support of the SSPA

Volume 2 TSPA (McNeish 2001 [DIRS 155023]) will result in some conservatism (overprediction) in the in-drift peak temperatures.

The uncertainty of the invert saturation, due to the thermal conductivity treatment, is most important for sub-boiling temperatures (all times for the LTOM and after centuries to about 1,000 years for the HTOM). The relationship between the invert temperature and the drip shield temperature will determine if condensation will occur primarily on the invert or on the drip shield. Since such condensation is a potential driver of waste package corrosion and of radionuclide transport after waste package failure, the location of the source of the condensation can be significant. The time of most significance is after the waste packages fail, and the current treatment is most realistic at those times. Thus, for in-drift water movement, the treatment of invert beams as low-conductivity degraded steel removes some of the uncertainty that could propagate to radionuclide release rates from the engineered barrier system.

5.3.2.4 Quantification of Uncertainty Using Process Models

As discussed in Section 5.3.2.3, some reductions or quantification of thermal-hydrologic uncertainties were included in the HTOM and LTOM for the SSPA Volume 2 (McNeish 2001 [DIRS 155023]) base case analyses. Other reductions or quantification of uncertainties were addressed using process-level models, including sensitivity studies. Some of the process-level analyses were conducted directly in support of the SSPA, while others had been conducted earlier. The results of the base case TSPA analyses and the process-level analyses provide 1) additional understanding of recognized uncertainties associated with thermal-hydrologic modeling as implemented in the multi-scale thermal-hydrologic model; 2) increased confidence in predicted temperature, relative humidity, and other measures of the in-drift environment over a range of thermal conditions bounded by the lower and higher temperature operating modes assumed; and 3) increased confidence in the results of the TSPA-SR.

This section describes the new and prior process-level analyses pertaining to the:

- Effects of forced ventilation efficiency and duration on in-drift temperatures and relative humidity (Sections 5.3.2.4.1, 5.3.2.4.2, and 5.3.2.4.3)
- In-drift humidity changes due to postclosure seepage or to near-field rock dryout caused by forced ventilation (Section 5.3.2.4.4)
- Treatment of natural convection and thermal radiation across the drift air gaps between the drift wall, drip shield, and waste package (Section 5.3.2.4.5)
- In-drift condensation distribution due to axial and cross-sectional temperature distributions (Section 5.3.2.4.6).

These analyses were conducted to better understand uncertainties and build confidence in the models supporting the TSPA for the HTOM and LTOM. They do not provide inputs directly to the SSPA Volume 2 TSPA (McNeish 2001 [DIRS 155023]).

5.3.2.4.1 Ventilation Efficiency from ANSYS and MULTIFLUX Calculations and from Scaled Tests

The MSTH model calculations in support of the TSPA-SR base cases (CRWMS M&O 2000 [DIRS 153246]) are described in Sections 5.3.1.3, 5.3.2.3, and 5.4. For the HTOM and LTOM, the calculations assumed a ventilation efficiency (the rate of heat removed by ventilating air divided by the rate of heat produced by the radioactive waste) constant in time and space. The HTOM calculations used a 50-year ventilation period with a constant ventilation efficiency of 70 percent. Because the heat source decreases with time, the ventilation efficiency improves as ventilation duration increases. Thus, the LTOM used a 300-year ventilation period with a constant ventilation efficiency of 80 percent. These values are rounded down from the time average of the ANSYS results described below for conservatism.

This section summarizes the ANSYS and MULTIFLUX calculations that support these values of ventilation efficiency, and the preliminary results of quarter-scale tests conducted to validate the calculations. The calculated and measured ventilation efficiencies are somewhat higher than those used in the TSPA base case calculations; therefore, the uncertainty in the TSPA calculations includes some bias toward warmer calculated temperatures than actually expected. The influence of such uncertainty and bias are quantified in Section 5.3.2.4.2.

ANSYS Calculations and Scaled Tests–For the two ventilation flow rates (10 and 15 m^3/s) for 200 years after emplacement, drift wall rock and the exit air temperatures were calculated at various time increments. ANSYS (V5.2 SGI) was used (CRWMS M&O 2000 [DIRS 120903]) with inlet air at 25°C and 0 percent relative humidity, an initial drift wall temperature of 70°C, and an initial waste package temperature of 70°C. The calculated results for the drift wall temperatures are shown in Figures 5.3.2.4.1-1 and 5.3.2.4.1-2. Drift wall temperatures presented are averages of the crown, spring line, and invert temperatures. The resulting air temperatures are shown in Figures 5.3.2.4.1-3 and 5.3.2.4.1-4.

Wall temperature (perimeter average) peaks within the first few years at the air inlet end of the drift and within five to fifteen years at the air discharge end of the drift. Air temperature peaks slightly later than wall temperature at the inlet end of the drift, but in the same time frame as the walls at the outlet end. For ventilation at 10 m^3/s, the maximum temperatures calculated occur at year 10 and are 94°C for the perimeter-averaged wall temperature at the exit end, with a corresponding maximum air temperature of 79°C. For ventilation at 15 m^3/s, calculated maximums occurred at the same time but were lower, 76°C for the wall and 64°C for the air.

The time histories of the rate of heat generation and removal for the 10 m^3/s and 15 m^3/s ventilation rates are presented in Figures 5.3.2.4.1-5 and 5.3.2.4.1-6. The heat generated is the same for both ventilation rates; it is the heat produced by average waste packages placed to produce a linear heat load of 1.54 kW/m in the drift. Heat removal by convective transfer from the waste package and the drift wall surface is included. Heat is removed by dry air; additional heat removal that will occur if moisture evaporates into the air is not addressed in the ANSYS calculations.

Peak heat removal rates occur within the 5 to 15 year time frame, but efficiency continues to increase due to natural decay in the magnitude of the heat source. Heat removed by ventilation at the rates of 10 and 15 m^3/s, respectively, was calculated by ANSYS to be 68 percent and 74 percent of the heat generated during the initial 50 years, 73 percent and 78 percent during the first 100 years, and 77 percent and 82 percent during a 200-year ventilation period.

A series of quarter-scale tests of ventilation efficiency was conducted in late 2000. A 1 m^3/s flow rate in a quarter-scale test is similar to a 15 m^3/s flow rate in a full-scale emplacement drift. Linear power loadings of 0.18 and 0.36 kW/m are similar to values of 0.72 and 1.44 kW/m in a full-scale drift. The calculated ventilation efficiencies (using ANSYS) of 74 percent for both of these tests (averaged over the 10-day test duration) are lower than the measured efficiencies of 86 percent and 83 percent for the two heating levels (Jurani 2001 [DIRS 155128]). The measured efficiencies of the test are based on measured temperature and flow rates (DTN: SN0106F3409100.003 [DIRS 155255]) and conversion to enthalpy change (Howard 2001 [DIRS 155132]). These tests are not yet complete, and several test condition and instrumentation issues are open. Nevertheless, the preliminary conclusion that the ANSYS calculations are conservative is reasonable, since some efficiency-enhancing effects were not included in the calculations.

MULTIFLUX Calculations–The MULTIFLUX model was developed by the University of Nevada, Reno under contract with the CRWMS M&O (Danko et al. 2001 [DIRS 154924]). The MULTIFLUX model couples a lumped parameter in-drift heat and mass transfer (airway) model to the NUFT code (V3.0), which models heat and mass transfer within the rock. NUFT is a TH computer code developed by Lawrence Livermore National Laboratory that is capable of analyzing mass transport coupled to energy transport by conduction, convection, and radiation in geologic media with multiple gas and liquid phases (including phase change). NUFT is also the software used in the MSTH model (see Section 5.2).

The MULTIFLUX model uses a number of initial NUFT runs to solve the heat and moisture mass transfer in the rock. These runs establish the relationship of rock temperature and partial vapor pressure to the heat and moisture flux at the drift wall surface. The MULTIFLUX software (V1.0) then uses the airway model to calculate heat and mass transfer within predefined drift segments. The airway model is based on computational fluid dynamics (CFD): it uses correlation-based heat transfer coefficients for natural and forced convection. At a given time step, the calculation using the airway model is repeated until the drift wall temperature, saturation, and humidity match the NUFT values at selected axial nodes. Then, the exit air temperature and humidity from a drift segment are used as the inlet conditions for the next segment. This process is repeated for successive drift segments until temperature, saturation, and humidity values have been calculated for the entire drift. The process is repeated for successive time steps.

Drift wall rock and exit air temperatures were calculated at various time increments for the two ventilation flow rates (10 and 15 m^3/s) at 200 years after emplacement. MULTIFLUX was used with inlet air at 25°C and 30 percent relative humidity, an initial drift wall temperature of approximately 24°C, and an initial waste package temperature of 25°C (BSC 2001 [DIRS 155025]). These two cases are similar to the ones simulated by the ANSYS model. The calculated drift wall temperatures (perimeter average) are shown in Figures 5.3.2.4.1-7 and 5.3.2.4.1-8. The resulting air temperatures are shown in Figures 5.3.2.4.1-9 and 5.3.2.4.1-10.

Drift wall temperature peaks within the first few years at the air discharge end of the drift. For a ventilation rate of 10 m^3/s, the maximum temperature calculated occurred at 2 to 5 years and was about 93°C. This result is very close to the ANSYS prediction of 94°C for the maximum wall temperature in 10 years. The corresponding maximum air temperature of 85°C calculated for the 10 m^3/s case is somewhat higher than the ANSYS result of 79°C. For 15 m^3/s, the maximum temperature calculated by MULTIFLUX occurred at 2 to 5 years and was approximately 71°C. This value is slightly lower than the ANSYS prediction of 76°C for the maximum wall temperature at 10 years. The corresponding maximum air temperature of 67°C calculated for the 15 m^3/s case using MULTIFLUX is somewhat higher than the ANSYS result of 64°C.

The rates of heat generated and removed with time for the 10 and 15 m^3/s ventilation rates are presented in Figures 5.3.2.4.1-11 and 5.3.2.4.1-12. Heat generated by the waste packages is the same for both ventilation rates; it is the heat produced by average waste packages that are placed to produce a linear heat load of 1.45 kW/m in the drift, an updated (smaller) value than used in the earlier ANSYS calculations. Heat removal by convection from the waste package and drift wall surfaces is included. Both sensible heat removal and latent heat removal from the emplacement drift by ventilation are included.

Heat removed by ventilation at the rates of 10 and 15 m^3/s, respectively, was calculated by MULTIFLUX to be 91 percent and 94 percent of the heat generated during the initial 50 years, 93 percent and 95 percent during the first 100 years, and 96 percent and 97 percent during a 200-year ventilation period. These rates of heat removal are significantly higher than predicted by the ANSYS calculations, which are 68 percent and 74 percent for 50 years, 73 percent and 78 percent for 100 years, and 77 percent and 82 percent for 200 years. The differences in predicted percentage of heat removal between the two models are 23 percent and 20 percent for 50 years, 20 percent and 17 percent for 100 years, and 19 percent and 15 percent for 200 years. The reasons for the higher heat removal prediction calculated by MULTIFLUX are partially due to the additional heat removal by natural convection and latent heat transfer, which were included in MULTIFLUX but not in ANSYS, due to the lower linear heat load (1.45 versus 1.54 kW/m) and due to a higher inlet pressure in the more recent MULTIFLUX calculations. The primary cause of the different ventilation efficiencies is likely to be the lumped parameter convection heat transfer coefficients used in the two models. The ANSYS calculations used 1.89 $W/m^2 \bullet k$ while the MULTIFLUX calculations used a value about three times larger. The correlation used in MULTIFLUX included roughness and entrance effects while the ANSYS calculation did not include these effects. The value of the ANSYS heat transfer coefficient was only about 20 percent larger than the natural convection heat transfer coefficient in an unventilated drift. The differences in heat removal need to be further studied and verified by the measurement data from the ventilation tests being conducted by the YMP.

The peak temperatures and efficiencies from the two models are summarized in Table 5.3.2.4.1-1. The inclusion of natural convection and latent heat in MULTIFLUX and the updated (lower) heat load result in higher efficiencies than for ANSYS. The smaller differences between drift wall and air temperatures in MULTIFLUX are consistent with a higher efficiency.

Relative humidity profiles calculated by MULTIFLUX at the 10 and 15 m^3/s ventilation rates are shown in Figures 5.3.2.4.1-13 and 5.3.2.4.1-14. As the air temperature increases along the emplacement drift, the relative humidity of air decreases because of the increase in saturation pressure (the denominator of the fraction that defines relative humidity). The relative humidity increases with ventilation duration as the air cools the emplacement drift and some water evaporates from the rock into the drift air. The lowest values of relative humidity (3 to 5 percent) occur at the end of the emplacement drift during the early (high temperature) period of ventilation. The highest values of relative humidity (32 to 34 percent) occur near the emplacement drift entrance at the maximum ventilation time.

The latent heat removal rates modeled by MULTIFLUX (Figures 5.3.2.4.1-11 and 5.3.2.4.1-12) are shown as the area between the "heat removed by ventilation" and "sensible heat removal by ventilation" curves. The results of integrating the area between the curves are shown in Table 5.3.2.4.1-2. The values shown in the table indicate that latent heat removal is a very small portion of the total heat removed by ventilation. This conclusion is also consistent with the hand calculations shown in Section 5.3.2.4.4.

Summary–Ventilation at rates of 10 to 15 m^3/s is capable of removing a large fraction (over 70 percent) of preclosure heat from emplacement drifts and controlling peak postclosure emplacement drift temperatures. Most of the heat removal is due to sensible heating of air as it moves across the heated waste packages and drift wall; only a small percent of heat removal by ventilation is due to the latent heat of water vaporized from the near-field rock.

Preliminary quarter-scale tests measured higher ventilation efficiencies than the ones calculated with the ANSYS model. The quarter-scale tests have not yet been modeled with MULTIFLUX. Based on the repository-scale calculations summarized in Table 5.3.2.4.1-1, the MULTIFLUX efficiencies should be closer to the test results than the ANSYS calculations. The difference in the convective heat transfer coefficients used in the two models is the primary source of the differences in the calculated ventilation efficiency.

Peak postclosure drift wall temperatures below 75°C are achievable at ventilation flow rates of 15 m^3/s and heat loads of 1.45 kW/m. Relative humidity during preclosure is dominated by the air temperature, with a minor influence due to water evaporating from the rock into the air (additional calculations of in-drift humidity effects due to evaporating water are shown in Section 5.3.2.4.4). Humidity remains below 35 percent during the entire preclosure period. As the air temperature increases along the emplacement drift, the relative humidity decreases. The lowest values of relative humidity (3 to 5 percent) occur at the end of emplacement drift during the early stage of ventilation. The relative humidity increases with time as ventilation cools the emplacement drift.

5.3.2.4.2 The Effect of a 10 Percent Uncertainty in Ventilation Efficiency and Assuming Ventilation Efficiency Is Time-Invariant

Preclosure temperatures and the postclosure peak temperature can be limited by removing heat from the system using preclosure ventilation. In Section 5.3.2.4.1, calculations and measurements of ventilation efficiency are summarized. Ventilation efficiency is defined as the rate of heat removed from the potential repository in the ventilation air divided by the rate of heat added due to radioactive decay of the emplaced waste. This subsection evaluates the sensitivity of thermal-hydrologic performance parameters (such as peak postclosure temperature) to the uncertainty in ventilation efficiency and to the assumption that ventilation efficiency is constant in time. The sensitivity was evaluated for both the HTOM and LTOM.

The LDTH submodel from the MSTH model (CRWMS M&O 2000 [DIRS 149862]) was used in the sensitivity analysis. The submodel results (Leem 2001 [DIRS 154996]) are suitable for determining the sensitivity of thermal-hydrologic parameters to the ventilation efficiency uncertainty. However, these sensitivity results do not include edge effects, variability of infiltration across the potential repository footprint, or three-dimensional in-drift phenomena. The MSTH results shown in Section 5.4, for the HTOM and LTOM base cases, should be used if values of thermal-hydrologic parameters are needed, rather than the sensitivity of those parameters to ventilation uncertainty.

The two-dimensional LDTH submodel was implemented (Leem 2001 [DIRS 154996]) for the L5C3 location in the potential repository footprint, as in a number of other sensitivity evaluations. This location has a thick cover of lower lithophysal rock (it is not near the interface with the middle non-lithophysal subunit above it). The surface infiltration rates (based on the methodology and input data in CRWMS M&O 2000 [DIRS 149862]) at this location are 5.7 mm/yr (present day climate, 0 to 600 years), 15.1 mm/yr (monsoonal climate, 600 to 2,000 years), and 23.2 mm/yr (glacial-transition climate beyond 2,000 yr). The submodel includes explicit thermal radiation between the drip shield and drift wall, and it applies a correlation-based effective thermal conductivity approach for natural convection heat transfer. The heat source in the model is volumetrically averaged within the volume enclosed by the drip shield. The invert in the model uses a thermal conductivity somewhat higher than the TSPA base cases described in Sections 5.3.1.3, 5.3.2.3, and 5.4. The sensitivity of the results to invert thermal conductivity were investigated in Section 5.3.1.4.10, which concluded that the results of sensitivity studies would not be significantly affected by the difference between the base case for the TSPA calculations and the base case for the two-dimensional submodel.

The HTOM calculations used the same initial linear heat loading, 1.35 kW/m, as the TSPA base case (Table 5.1-1). The two-dimensional base case used for the HTOM sensitivity calculations also used the same ventilation parameters as the TSPA base case, 50 years of forced ventilation at an assumed heat removal efficiency of 70 percent. Similarly, the sensitivity base case used for the LTOM sensitivity calculations used the same values as the TSPA base case: 1.13 kW/m initial linear heat loading and 300 years of forced ventilation at an assumed efficiency of 80 percent.

The thermal hydrology sensitivity calculations focused on the effect of the ventilation efficiency on in-drift thermal-hydrologic conditions. In addition to the base case for each operating mode, constant ventilation efficiency cases were run in which the ventilation efficiency was 10 percent higher or 10 percent lower than the base case. The base case ventilation efficiency used in the sensitivity calculation is an averaged value throughout the pre-closure period, and the +/-10 percent value could consider local and temporal changes in the ventilation efficiency. Because the ventilation efficiency was determined as a function of time using the ANSYS (V5.2) software, the time-dependent ventilation efficiency was also considered in the LDTH sensitivity analysis for each operating mode, HTOM and LTOM (Section 5.3.2.4.5). The time-dependent cases are denoted, f(t), in the results below. Finally, it was noted that the time-averaged efficiency for each of the time-dependent cases was actually somewhat higher than the base case;

therefore, one additional case was run for each operating mode. The additional case used a constant ventilation efficiency equal to the average of the time-dependent efficiency, to allow direct comparison of the effect of time-dependency on in-drift thermal-hydrologic parameters.

Figure 5.3.2.4.2-1 shows the time-dependent ventilation efficiency for the HTOM and LTOM. These curves were developed from the *Ventilation Model* (CRWMS M&O 2000 [DIRS 120903]). The time-dependent values for the LTOM after the first 50 years were calculated from the ratio between the HTOM and LTOM efficiencies, since the forced ventilation efficiency values provided for the LTOM linear heat loading were only for 0 to 50 years. The predicted ventilation efficiency values for the LTOM beyond 50 years are probably conservative (Section 5.3.2.4.1), since the efficiency of ventilation is increased in a low temperature condition, and temperatures for the LTOM decrease with time during the 50 to 300-year period.

Higher-Temperature Operating Mode Results–The use of a ventilation efficiency in the LDTH submodel reduces the heat available to be transported from the waste packages into the near-field rock. Figure 5.3.2.4.2-2 shows the time history of available waste package heat for the constant base case and time-dependent f(t) ventilation cases. The total heat (available for transport plus removed by ventilation) is also shown.

The drip shield top and drift wall crown peak postclosure temperatures of the HTOM are well above the boiling point, 96°C, for all the ventilation efficiency cases (Figures 5.3.2.4.2-3 and 5.3.2.4.2-4). Increasing the ventilation efficiency across the 20 percent range investigated (60 percent to 80 percent), decreases the peak postclosure temperatures of the drip shield and drift wall crown by about 14°C each. The postclosure temperature results for the time-dependent ventilation efficiency case are similar (within 1°C) to those for the corresponding constant ventilation efficiency (73 percent). As the drift wall and drip shield temperatures increase, the driving force for heat transfer to the ventilation air increases, causing the ventilation efficiency to increase and the rock and drip shield temperatures to decrease. During the preclosure period, high waste package temperature is less significant than during postclosure because of the short duration of high temperature and because of the low humidity during preclosure.

The relative humidity histories at the same locations as the temperature histories are shown in Figures 5.3.2.4.2-5 and 5.3.2.4.2-6. For constant (in time and space) ventilation efficiencies, the time for relative humidity to increase to 50 percent decreases by about 120 years and 80 years for the drip shield top and drift wall crown, respectively, as ventilation efficiency increases from 60 percent to 80 percent. The shorter time to return toward ambient humidity values is due to less heating of the near-field rock when ventilation is more effective. For the time-dependent ventilation efficiency case, there is a much lower humidity minimum, consistent with the higher preclosure temperature.

The saturation of the invert decreases from the initial condition of about 10 percent to a dry value within 10 years for all the ventilation efficiency cases (Figure 5.3.2.4.2-7). The dry conditions persist well beyond the closure of the potential repository. The increase of invert saturation back to ambient values, beyond 1,000 years, is shown in Section 5.4.1.

A summary of the thermal hydrology sensitivity modeling results is presented in Table 5.3.2.4.2-1.

Lower-Temperature Operating Mode Results–Figure 5.3.2.4.2-8 shows the time history of available waste package heat for the constant and time-dependent ventilation cases. The total heat (available for transport plus removed by ventilation) is also shown.

The drip shield top and drift wall crown peak postclosure temperatures of the LTOM are below 85°C (Figures 5.3.2.4.2-9 and 5.3.2.4.2-10). Increasing the ventilation efficiency across the 20 percent range investigated (60 percent to 80 percent), decreases the peak postclosure temperatures of the drip shield and drift wall crown by 7°C. The postclosure temperature results for the time-dependent ventilation efficiency case are similar (within 1°C) to those for the corresponding constant ventilation efficiency (83 percent). During the preclosure period, the relative humidity of the ventilation air will be less than 30 percent, so that corrosion of the drip shield and waste package is unlikely. Nevertheless, further study is warranted of the ventilation efficiency during the transient period of the first five to ten years when components reach quasi-steady temperatures. It is encouraging that the transient period in the initial quarter scale tests of ventilation efficiency (DTN: SN0106F3409100.003 [DIRS 155255]) was faster than the model calculations (CRWMS M&O 2001 [DIRS 155328]). Continued test results and more sophisticated calculations will be used, in support of a potential license application, to better define the preclosure temperature spike duration and magnitude.

Values of relative humidity for the drip shield top decrease to only about 75 percent during the preclosure period for the constant efficiency cases, and to about 40 percent for the time-dependent efficiency cases (Figure 5.3.2.4.2-11). However, it should be noted that these values are based on two-dimensional equilibration of stagnant drift air with the near-field rock, which ignores the humidity influence of the ventilation air. During the preclosure period, the relative humidity will be set by the ventilation air inlet relative humidity (Section 5.3.2.4.4). The postclosure minimum for drip shield top humidity is about 60 percent. At the drift wall, there is essentially no reduction in humidity in the LTOM sensitivity calculations. The saturation of the lower, center region of the invert shows a similar pattern for the LTOM (Figure 5.3.2.4.2-12) and the HTOM (Figure 5.3.2.4.2-7). The initial saturation of about 10 percent decreases to a minimum that is totally dry for some of the ventilation efficiency cases, and partly dried for others. Beyond 50 years, however, the continuing ventilation of the LTOM removes sufficient heat that the invert begins to rewet, reaching saturation of 1.5 to 4.5 percent, depending on the ventilation efficiency. Then, when the potential repository is closed, there is a postclosure drying of the invert. The increase of invert saturation back to ambient values, beyond 1,000 years, is shown in Section 5.4.2.

A summary of the thermal hydrology sensitivity modeling results is presented in Table 5.3.2.4.2-2.

Summary–In-drift temperatures are sensitive to ventilation efficiency, with a 20 percent decrease in efficiency resulting in a drip shield peak postclosure temperature increase of 14°C for the HTOM and 7°C for the LTOM. The transient period during the first five to ten years is expected to receive further study in calculations and testing to support a potential license application considering the mass transfer by the pre-closure ventilation. Operational procedures, including partial loading of drifts to spread out the transient period, are also being considered to mitigate the potential preclosure temperature spike.

5.3.2.4.3 The Effect of Calculating Temperatures Based on Simultaneous Emplacement of Appropriately Aged Waste Packages

The MSTH model (CRWMS M&O 2000 [DIRS 149862]) focuses on temperature, saturation, and humidity during the postclosure period. This emphasis allows a simplified approach for the waste emplacement period of the preclosure phase of a potential repository. The simplification is to emplace all waste simultaneously, but use thermal decay curves that are appropriate for the age of waste as it is sequentially emplaced in accordance with an assumed waste acceptance schedule. For the LTOM, the TSPA used a 300-year ventilation period. The TSPA scenario does not specify if this period is an average (with some waste packages receiving more and some receiving less ventilation duration), the duration for the initial waste packages emplaced, or the duration for the final waste packages emplaced. One scenario for waste emplacement assumes a 22-year emplacement period. In this section, the base case ventilation duration is varied by ±22 years to determine the effects of the uncertainty of ventilation duration on in-drift TH parameters in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) scenario. This emplacement period is taken from the *Reference Design Description for a Geologic Repository* (CRWMS M&O 2000 [DIRS 151967], Table 2). The first two years of the scenario, which had low rates of waste emplacement, were not included. The waste emplacement rates implicit in this scenario represent assumptions used only for this analysis.

This sensitivity analysis (Leem 2001 [DIRS 154996]) employed the LDTH submodel using the same implementation methods described in Section 5.3.2.4.2.

The base case for the sensitivity analysis is the LTOM base case design, with a 1.13 kW/m initial linear heat loading and 300 years of forced ventilation at an assumed (constant) ventilation efficiency of 80 percent (Table 5.1-1).

Results–The peak postclosure temperatures at the top of the drip shield and the crown of the drift wall are well below 85°C for all three ventilation duration cases (Figures 5.3.2.4.3-1 and 5.3.2.4.3-2). The peak postclosure temperatures of the drip shield and drift wall decrease 2 to 3°C as the ventilation duration increases from 278 years to 322 years. An additional interpretation of these results is that aging of 20 to 40 years for a 300-year ventilation period would not produce a significant (greater than a few degrees centigrade) reduction in peak postclosure temperatures.

Values of relative humidity for the drip shield top never decrease below 60 percent in all three ventilation duration cases (Figure 5.3.2.4.3-3). At the drift wall, the humidity remains nearly 100 percent at all times.

In all three ventilation durations investigated, the saturation at the lower center of the invert dries within a few decades during the preclosure period, rewets to about 3 percent saturation by potential repository closure, then quickly dries again (Figure 5.3.2.4.3-4). Section 5.4 shows the subsequent rewetting of the invert beyond 1,000 years for the LTOM base case. The sensitivity of the in-drift TH parameters to ventilation duration in the LTOM is summarized in Table 5.3.2.4.3-1.

Summary–In the LTOM, the duration of ventilation (300 years) is long enough that the TH results are insensitive (within a few degrees centigrade of peak in-drift temperatures) to variations of plus or minus a few decades of ventilation duration.

5.3.2.4.4 The Influence of Near-Field Rock Dryout Due to Forced Ventilation on In-Drift Relative Humidity

The moisture contained in the host rock, if evaporated into the ventilation air, can influence the temperature and humidity conditions in an emplacement drift. Determination of water movement in the surrounding rock mass during preclosure ventilation requires complex models (e.g., MULTIFLUX, described in Section 5.3.2.4.1) to simulate the coupled heat and mass transfer processes.

To illustrate the overall effect of water removal by ventilation on the psychrometric environment in the drift, a constant rate of water removal from the rock was assumed in two numerical examples. Both examples include the effects of vaporization of near-field water on in-drift relative humidity and heat removal efficiency. The first example considers the initial dryout of the rock by the ventilating air. MSTH model (CRWMS M&O 2000 [DIRS 149862]) results presented later in this subsection, and limited measurements in the Exploratory Studies Facility (ESF), support a dryout depth of several meters. The observation of ventilation-caused dryout in the ESF supports dryout times less than a few years. To obtain a high-side but realistic bounding value of dryout-caused influx of water into the ventilation air, a dryout depth of 3 meters during a time span of 6 months was used in the example calculation. The second example considers continuing evaporation of water into the ventilating air, with the water furnished by percolation flux moving downward through the unsaturated zone and being intercepted by the dryout zone (about two drift diameters wide, from the first example). Recognizing that the results of this steady-state influx of water will be less than the initial dryout-period influx, a typical flux value of 10 mm/yr was used; the insensitivity of the resulting humidity to the influx (reported below) supports selection of a typical, rather than lower bound, value. The LDTH submodel of the MSTH model was used to investigate the influence of preclosure rock dryout on in-drift temperature and humidity. The submodel was implemented using assumed in-drift gas pressure and composition to drive movement of water vapor from the rock into the drift.

Finally, the LDTH submodel was used to investigate the influence of postclosure seepage of liquid water on in-drift temperature and humidity. The submodel was implemented using assumed seepage of liquid water into in-drift locations.

Initial Dryout–Ventilation air will initially evaporate existing water from the rock. As the depth of evaporation increases, the evaporated water must move through larger and larger regions of previously dried rock. In this example calculation, it is assumed that the initial dryout period is about 6 months and that the dryout extends to a depth of 3 m beyond the drift wall. It is assumed that the air enters the drift at a rate of 15 m^3/s, a temperature of 25°C, and a relative humidity of 30 percent. Finally, it is assumed that the air is heated by the waste packages and drift walls to a temperature of 45°C as it travels through the first 500 m of the drift.

Based on the intake air parameters, the water vapor pressure at the drift inlet depends on the temperature and relative humidity of the inlet (Hartman 1982 [DIRS 128009], pp. 596 to 597)

$$
\begin{aligned}
p_{v1} &= R_1\{0.6105\exp[17.27t_{ao1}/(t_{ao1}+237.3)]\} \\
&= 30\%\{0.6105\exp[17.27\times 25/(25+237.3)]\} = 949.9\,Pa
\end{aligned}
$$

where

p_{v1} = water vapor pressure at the emplacement drift inlet (Pa)
R_1 = relative humidity of intake air at emplacement drift inlet (percent)
t_{ao1} = air temperature at the emplacement drift inlet (°C)

The specific humidity (water-air ratio) of the intake airflow is (Hartman 1982 [DIRS 128009], p. 597):

$$
\begin{aligned}
\omega_1 &= 0.622\times p_{v1}/(p_b - p_{v1}) = 0.622\times 949.9/(88720-949.9) \\
&= 0.00673\ \text{(kg water)/(kg air)}
\end{aligned}
$$

where

ω_1 = specific humidity of intake air (kg water)/(kg air)
p_b = barometric pressure at potential repository level (88,720 Pa; CRWMS M&O 1999 [DIRS 106794], p. 6, Section 3.4).

The rate of water (or moisture) entering the emplacement drift with the intake airflow is:

$$W_1 = Q\times\rho_1\times\omega_1 = 15\times 1.0561\times 0.00673 = 0.10664\ \text{kg water/s}$$

where

W_1 = rate of moisture entering drift with intake airflow (kg water/s)
Q = airflow rate at emplacement inlet (m^3/s)
ρ_1 = density of air at potential repository level (1.0561 kg/m^3) (CRWMS M&O 1998 [DIRS 105230], p. II-2, 3530 ft altitude, 70°F).

For the first 500 m of an emplacement drift with a 5.5-m diameter, the volume of a 3-m annulus of rock is:

$$V_r = 500\times(\pi/4)\times[(5.5+6)^2 - (5.5)^2] = 40{,}055\ \text{m}^3$$

When the rock volume, V_r, is multiplied by an average matrix porosity of ϕ = 11.3 percent, an initial matrix saturation of about S = 90 percent, and ρ_w = 1,000 kg/m^3 density of water, the water content of the dryout zone is calculated to be 4,074,000 kg. To remove this amount of water in a period of 6 months, the average rate of water entering the ventilation airflow is:

$$W_2 = V_r \times \phi \times S \times \rho_w \left(365/2 \times 24 \times 3600\ s\right)$$
$$= 0.2583\ \text{kg water/s}$$

This water addition into the ventilation airflow will increase the specific humidity (water-air ratio) to:

$$\omega_2 = (W_1 + W_2)/(Q \times \rho_1)$$
$$= (0.10664 + 0.2583)/(15 \times 1.0561) = 0.02304\ kg\ water/kg\ air$$

Compared with ω_1 = 0.00673 kg water/kg air at intake, the water content of the airflow at 500 m more than tripled because of moisture removal by ventilation during dryout of the first 500 m of the wall rock.

For ω_2 = 0.02304 kg water/kg air, the water vapor pressure of airflow 500 m downstream of the drift inlet is (Hartman 1982 [DIRS 128009], p. 597):

$$p_{v2} = p_b/[(0.622/\omega_2) + 1]$$
$$= 88720/[(0.622/0.02304) + 1] = 3169\ Pa$$

The saturation pressure (p_{s2}) of air at the 500-m point, where the air temperature (t_{ao2}) = 45°C, is (Hartman 1982 [DIRS 128009], p. 596):

$$p_{s2} = 610.5 \exp[17.27 t_{ao2}/(t_{ao2} + 237.3)]$$
$$= 610.5 \exp[17.27 \times 45/(45 + 237.3)] = 9578\ Pa$$

The relative humidity (R_2) of the airflow at the 500-m point is (Hartman 1982 [DIRS 128009], p. 597):

$$R_2 = (p_{v2}/p_{s2}) \times 100\%$$
$$= (3169/9578) \times 100\% = 33\%$$

If no moisture was removed from the drift wall, the relative humidity at the 500-m point due to temperature change alone would be (p_{v1}/p_{s2}) = 9.9 percent.

The contribution to heat removal of the latent heat of water vaporization during the dryout period can also be calculated. First, the average rate of water removal from the wall rock of a 500-m drift segment is placed on a per-meter-of-drift basis:

$$W_2' = (0.2583\ kg\ water/s \div 500\ m = 0.0005167\ kg\ water/(m\ s)$$

During the dryout period, the water in the host rock, which has an initial temperature of 25°C, is heated and vaporized into the ventilation air stream. For an increase in air temperature to 45°C at the 500-m point, the lineal power (heat) removal due to sensible and latent heating is:

$$
\begin{aligned}
H_{water} &= W_2^{'}\{c_{p1}(45°C - 25°C) + h_{vaporization}\} \\
&= 0.0005167\ kg/m \bullet s \times \{4.178\ kJ/kg \bullet C \times (45°C - 25°C) + 2418.42\ kJ/kg\} \\
&= 1.29\ kJ/m \bullet s \\
&= 1.29\ kW/m
\end{aligned}
$$

where c_{p1} is the specific heat of water (kJ/kg•C).

For an average temperature of ((45+25)/2) = 35°C, the value of c_{p1} is 4.178 kJ/kg•C and the value of $h_{vaporization}$ (heat of vaporization) is 2418.42 kJ/kg (linearly interpolated from Incropera and DeWitt 1985 [DIRS 114109], p. 774).

Compared with the initial linear heat loadings of 1.35 and 1.13 kW/m (see Table 5.1-1) for the HTOM and LTOM, the lineal latent heat removal during the dryout period is significant.

Evaporation of Percolation Flux–Following the initial dryout of the 3-m rock annulus, it is assumed that a percolation flux of 10 mm/yr will be intercepted over an 11.5 m-wide path (a 3-m dryout zone, a 5.5-m drift diameter, and a 3-m dryout zone combined). All percolation water entering this zone is assumed to be removed by the ventilation air in the drift. The rate of water removal is:

$$
\begin{aligned}
W_3 &= Q_p \times A \times \rho_w \\
&= (10\ \text{mm/yr} \times 0.001\ \text{m/mm} \div 31536000\text{s/yr}) \times (500m \times 11.5m) \times 1000\ kg/m^3 \\
&= 0.001823\ \text{kg water/s}
\end{aligned}
$$

where

W_3 is the rate of percolation water evaporation into the drift air
Q_p *is* the percolation flux
A is the area of percolation flux intercepted
ρ_w is the density of water

This is only about 1.7 percent of the water removal rate during the dryout period. Using the same methods as the preceding example, the water addition rate can be converted to an air relative humidity. Because the percolation water addition is small compared to the initial water content of the air, the resulting relative humidity of the airflow at the 500-m point will be 10.01 percent, similar to the 9.9 percent value if no water were added due to steady percolation.

The contribution to heat removal of the latent heat of water vaporization due to percolation after the near-field rock dryout period can be calculated in a manner similar to the dryout period example above. The water removal rate calculated above, 0.001823 kg water/s, corresponds to 0.000003646 kg water/(m•s). Using this rate, the latent plus sensible heat removal due to water is calculated to be 9.1 W/m, only about one percent of the initial linear heat loadings of 1.35 and 1.13 kW/m for the HTOM and LTOM. This contribution of water latent plus sensible heating to ventilation heat transfer due to vaporization of percolation flux is similar to the MULTIFLUX results presented in Section 5.3.2.4.1.

Effect of Preclosure Dryout of Near-Field Rock on Postclosure In-Drift Temperature and Relative Humidity–The dryout of the host rock surrounding emplacement drifts due to ventilation with relatively dry air results in a reduction in the thermal conductivity in the dryout zone. As is shown in Table 5.3.1.4.8.1, thermal conductivity decreases with liquid saturation. The preclosure LDTH submodels used in the MSTH model do not account for preclosure dryout and the influence of that dryout on reducing thermal conductivity in the host rock around emplacement drifts. Thus, the postclosure LDTH submodels used in the MSTH model start with liquid saturation in the host rock being very close to ambient conditions. Note that for the thermal-hydrologic model calculations conducted for this section, the ambient liquid saturation is 0.94 in the matrix continuum, Figure 5.3.2.4.4-1). In this section, we investigate whether explicitly accounting for rock dryout during the preclosure period significantly influences predicted thermal-hydrologic conditions during the postclosure period. The LDTH submodel at the L5C3 location was used to investigate this sensitivity. The location and infiltration boundary conditions for the two-dimensional submodel were the same as those described in Section 5.3.2.4.2. Four different cases (called Cases 1, 2, 3, and 4) are considered for both the HTOM and LTOM, with each case having different assumptions about thermal-hydrologic conditions within the emplacement drifts during the preclosure ventilation period.

For each of the four cases and for both of the operating modes, the model was implemented in three steps. The first step was to run the model during the preclosure period to obtain the drift-wall temperature history, using the base-case ventilation efficiencies: 70 percent for 50 years for the higher-temperature operating mode and 80 percent for 300 years for the lower-temperature operating mode. Section 5.3.2.4.2 discusses the sensitivity of thermal-hydrologic behavior to uncertainty in the ventilation efficiency. The second step was to repeat the preclosure calculation for the rock portion of the model, using the Step-One drift-wall temperature history and an assigned gas boundary condition at the drift wall.

In Step Two, the gas boundary condition was assigned to have a gas-phase pressure of 99 percent of ambient pressure and a relative humidity of 30 percent during the preclosure ventilation period for Case 1. A relative humidity of 30 percent is close to the mean annual relative humidity at the ground surface at Yucca Mountain. The psychrometric properties of the intake air for the ventilation of the emplacement drifts are summarized in (BSC 2001 [DIRS 155246], Table XXVII-1). The emplacement drifts are ventilated by pulling (rather than pushing) air, which causes the gas-phase pressure in the ventilated drifts to be reduced by a maximum of about 1 percent relative to ambient conditions (CRWMS M&O 2000 [DIRS 154176], p. 22). Cases 2 and 3 assign different values of either gas-phase pressure or relative humidity, while Case 4 uses different ventilation efficiencies than in Cases 1, 2, and 3. Thus, the ventilated emplacement drift functions as a sink for the humid gas in the host rock due to the lower gas-phase pressure and lower water vapor content of the in-drift air compared to the air in the near-field rock. Note that under ambient conditions, relative humidity in the host rock is greater than 99 percent.

The final preclosure distributions of temperature, liquid saturation, gas-phase pressure, and relative humidity in the host rock from Step Two become the initial rock conditions for the Step-Three postclosure calculation. Thus, Step Three captures the influence of preclosure dryout of the host rock. Step Three is similar to Step One in that the line-averaged heat-generation rate of the waste packages is represented in the LDTH submodel, rather than representing the influence of this heat generation with a specified boundary temperature as was done in Step Two. During the postclosure period, 100 percent of the heat generated by waste packages is represented in the LDTH model. Figures 5.3.2.4.2-2 and 5.3.2.4.2-8 show the heat-generation histories for the higher- and lower-operating modes, respectively.

This three-step process was repeated for Cases 2, 3, and 4 for both the higher- and lower-temperature modes. Case 2 is the same as Case 1 except relative humidity in the drift is assigned to be 5 percent (instead of 30 percent) during the preclosure period. The value of 5 percent corresponds to the minimum relative humidity of the ventilation air (4.77 percent), which is calculated to occur at 10 years (BSC 2001 [DIRS 155246]). A relative humidity of 5 percent represents an extreme lower bound for the in-drift relative humidity conditions during the ventilation period. Case 3 is the same as Case 1 except gas-phase pressure in the drift is assigned to be 95 percent of ambient during the preclosure period. Case 4 is the same as Case 1 except the ventilation efficiencies are assigned to be 60 percent for 50 years for the HTOM and 70 percent for 300 years for the LTOM (10 percent less than the other cases for both operating modes).

Figure 5.3.2.4.4-1 shows the lateral extent of host-rock dryout at the end of the preclosure ventilation period for Case 1. At the time of closure, liquid saturation in the matrix is reduced to about 0.5 at distances of 3 m and 1 m laterally away from the drift wall, for the higher- and lower-temperature operating modes, respectively.

For the higher-temperature operating mode, Figure 5.3.2.4.4-2 compares the results of Case 1 to those of the base-case L5C3 LDTH submodel (the base case neglects the influence of rock dryout during the preclosure period). The results of the base-case L5C3 LDTH submodel, together with those of the LDTH submodels at the 32 other geographic locations in the potential repository, are included in the generation of the MSTH model results described in Section 5.4.1. Figure 5.3.2.4.4-2 shows that Case 1 and the base case result in almost identical postclosure temperature at the drift wall and drip shield, relative humidity at the drip shield, and liquid saturation in the invert and at the drift wall. The preclosure dryout predicted for Case 1 has a negligible effect on postclosure thermal-hydrologic conditions around the drift. The rapid increase in temperatures (above the boiling point of water) following the cessation of ventilation generates a much larger dryout zone than that generated during the preclosure ventilation period, thereby overwhelming the influence of the preclosure dryout calculated in Step Two of the three-step calculation.

For the lower-temperature-operating mode, Figure 5.3.2.4.4-3 compares the results of Case 1 to those of the base-case L5C3 LDTH submodel, (the base case neglects the influence of rock dryout during the preclosure period). The results of the base-case L5C3 LDTH submodel, together with those of the LDTH submodels at the 32 other geographic locations in the potential repository, are included in the generation of the MSTH model results described in Section 5.4.2. Figure 5.3.2.4.4-3 shows that Case 1 and the base case result in almost identical postclosure temperature at the drift wall and drip shield, relative humidity at the drip shield, and liquid saturation in the invert and at the drift wall. The preclosure dryout predicted for Case 1 has a negligible effect on postclosure thermal-hydrologic conditions around the drift. Rewetting of the host rock (primarily by matrix imbibition) requires about one hundred years after closure. However, peak temperatures at the drift wall and drip shield occur even later, two to three hundred years after closure for the lower-temperature operating mode, and are not affected by the inclusion of preclosure dryout in the LDTH submodel calculation. Because the dryout zone (which corresponds to the region of reduced thermal conductivity in the host rock) has collapsed prior to the occurrence of peak temperatures for the LTOM, rock dryout has a negligible influence on peak temperatures, as well as on other thermal-hydrologic conditions in the emplacement drifts.

Figure 5.3.2.4.4-4 compares the lateral extent of host-rock dryout at the end of the preclosure ventilation period for the HTOM and LTOM for Cases 1, 2, 3, and 4. The lower input value of relative humidity in the drift for Case 2 (5 percent) compared to Case 1 (30 percent) causes the lateral extent of dryout to extend further into the rock. The lower input value of gas-phase pressure in the drift for Case 3 (95 percent of ambient) compared to Case 1 (99 percent of ambient) causes the lateral extent of dryout to extend further into the rock. Case 4, which uses a lower ventilation efficiency than Case 1, results in higher temperature at the drift wall during the preclosure ventilation period and causes the lateral extent of dryout to extend further into the rock. For all three cases (2-4), the influence of this effect is greater for the higher-temperature-operating mode than for the lower-temperature operating mode. Summarizing, the lateral extent of host-rock dryout increases with decreasing relative humidity and gas-phase pressure in the drift and it increases with increasing drift-wall temperature. Figure 5.3.2.4.4-5 compares Cases 1, 2, 3, and 4 for the HTOM. Although Cases 1, 2, and 3 produced slightly different lateral extents of preclosure dryout, they result in almost identical postclosure temperature at the drift wall and drip shield, relative humidity at the drip shield, and liquid saturation in the invert and at the drift wall. Recall that Case 1 has a virtually identical temperature, liquid saturation, and relative humidity conditions as in the base-case LDTH submodel that ignored the influence of preclosure dryout. Therefore, Cases 1, 2, and 3 result in the same temperature, liquid saturation, and relative humidity conditions as in the base-case LDTH submodel that neglects preclosure dryout. Case 4 results in slightly higher temperatures, and in slightly lower liquid saturation and relative humidity, than in Cases 1, 2, and 3. The primary cause of the higher temperature and lower liquid saturation and relative humidity in Case 4 is that it utilized a lower heat removal efficiency during the preclosure ventilation period, resulting in higher temperatures at the beginning of the postclosure period. The secondary cause of the higher temperatures is the large dryout zone that results in a larger region of reduced thermal conductivity, causing postclosure temperatures to be somewhat higher.

Figure 5.3.2.4.4-6 compares Cases 1, 2, 3, and 4 for the lower-temperature-operating mode. Cases 1, 2, and 3 produce essentially identical postclosure temperature at the drift wall and drip shield, relative humidity at the drip shield, and liquid saturation in the invert and at the drift wall. Recall that Case 1 has similar temperature, liquid saturation, and relative humidity conditions as in the base-case LDTH submodel that ignored the influence of preclosure dryout. Therefore, Cases 1, 2, and 3 result in the same temperature, liquid saturation, and relative humidity conditions as in the base-case LDTH submodel that neglects preclosure dryout. Case 4 also results in similar liquid saturation and relative humidity conditions; however, Case 4 results in slightly higher temperatures than in the other cases. The cause of the higher temperature in Case 4 is that it utilized a lower heat removal efficiency during the preclosure ventilation period, resulting in higher temperatures at the beginning of the postclosure period.

Effect of Postclosure Seepage on In-Drift Temperature and Relative Humidity–Seepage into the drift was not predicted to occur for most of the range of infiltration flux conditions considered in the TH model calculations developed in the *Water Distribution and Removal Model* (CRWMS M&O 2001 [DIRS 152016]) and used in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]). One reason for the low prediction of drift seepage is the assumption of a uniform fracture continuum within each hydrostratigraphic unit. This assumption is equivalent to assuming no drift-scale heterogeneity of fracture properties in the host rock, reducing the tendency for drift seepage. The two-dimensional nature of the current LDTH submodel also contributes to the lack of heterogeneity in the horizontal direction.

To overcome the tendency of the LDTH models to predict little or no seepage, a sensitivity study was conducted during the preparation of the *Water Distribution and Removal Model* (CRWMS M&O 2001 [DIRS 152016]). The LDTH submodel was modified to impose seepage within the drift for a design and operating point similar to the HTOM. The model added the seepage uniformly over the upper drip shield surface and drift floor (i.e., the upper invert surface) between the base of the drip shield and the intersection of the drift floor and lower drift wall. Sources of liquid water were specified at each of the gridblocks overlying the drip shield or drift floor, including the gridblock overlying the column of gridblocks adjacent to the vertical side of the drip shield.

Three values of seepage percentage were considered: 0, 3, and 30 percent. For this sensitivity study, the seepage percentage was taken to be the percentage of the incident percolation flux in the host rock that directly overlies the invert on which the seepage was imposed. The invert lateral width of 3.2 m (CRWMS M&O 2000 [DIRS 149862], Figure 6-2) is less than the 5.5-m drift diameter. Because the LDTH submodels have boundary conditions that prevent lateral diversion of water, the percolation flux in the host rock (averaged across the model domain) is equivalent to the average infiltration flux specified at the top of that LDTH submodel location. The L4C4 location used for this sensitivity study was near the geographic center of the potential repository, and it experiences slightly higher than average infiltration (and percolation) flux conditions. The infiltration flux was calculated to be 10.13, 28.88, and 42.00 mm/yr for the present-day, monsoonal, and glacial climate states, respectively (CRWMS M&O 2001 [DIRS 152016], Table 5-4). For the 30 percent-seepage case, the resulting seepage fluxes were 3.04, 8.66, and 12.6 mm/yr, respectively, calculated over a footprint that is 3.2214 m wide.

To avoid artificial addition or subtraction of sensible heat from the drift due to seepage, an assumption was made that the water seeping into the drift had equilibrated with the host rock temperature at the crown of the drift. A maximum allowable temperature of 96°C was set to assure that the seepage flux entered the drift as liquid water. This assumption was implemented by extracting the temperature history for the host rock at the crown of the drift for the case with 0 percent seepage (i.e., no prescribed seepage into the drift). The temperature history was used to linearly interpolate an enthalpy history from the steam tables (Keenan et al. 1969 [DIRS 134666]).

Figure 5.3.2.4.4-7 shows the influence of drift seepage on temperature and relative humidity at the drip shield. Drift seepage flux is seen to have negligible influence on drip-shield temperature and relative humidity.

Summary–The volume of water that can enter the ventilation air during dryout of the near-field rock is sufficient to triple the relative humidity of the exiting ventilation air (from about 10 percent to 33 percent). During the dryout period (based on the assumed dryout rate), the latent heat of the vaporizing water can remove all of the heat flux from the waste packages. This is a higher value than the latent heat removed in ventilation air as calculated with MULTIFLUX in Section 5.3.2.4.1, indicating that much of the mobilized moisture may be removed as vapor may be through fractures in the mountain, rather than in the ventilation air.

After dryout of the near-field rock, the vaporization of percolating water into the ventilation air is slow enough that only small changes in ventilation air humidity and cooling rate are calculated. The MULTIFLUX results summarized in Section 5.3.2.4.1 corroborate the hand calculations.

After closure, most in-drift temperature and humidity histories are not significantly influenced by the low saturation of near-field rock dried during the ventilation period. In the LTOM, the saturation at the drift wall does not rewet for about a century after ventilation ceases; however, based on these two-dimensional calculations, the low saturation does not significantly affect in-drift temperatures or relative humidity at the drip shield.

Finally, if seepage water equilibrates thermally with the near-field rock prior to seeping, direct imposition of seepage water into in-drift zones does not significantly affect in-drift temperatures or humidity at the drip shield.

5.3.2.4.5 Use of an Effective In-Drift Heat Transfer Coefficient to Represent Radiation in the Line-Source Drift-Scale Thermal-Hydrologic and the Discrete-Source Drift-Scale Thermal Submodels

An effective thermal conductivity applied to the in-drift air elements in the drift-scale models of the potential repository can be used to approximate complex modes of heat transfer, including thermal radiation and natural convection, by using a standard Fourier law of heat conduction approach. The effective thermal conductivity parameter governs the calculated rate at which heat is transferred from the heat source (by all relevant modes of heat transfer) to the drift wall or from the drip shield to the drift wall after closure of the potential repository. There are two advantages to using an effective thermal conductivity in the models. First, complex modes of heat transfer can be approximated by models of the potential repository that are currently incapable of handling the necessary transport mechanisms required by a particular mode of heat transfer (i.e., highly turbulent natural convection in an open cavity). Second, applying this method greatly reduces model run times.

It is noted that the effective thermal conductivity is temperature dependent. As such, it is necessary to have an a priori knowledge about the temperatures so that an effective parameter can be developed. Since this is a potential limitation in the development of the effective parameter, the sensitivity of the process-level models to effective thermal conductivity developed with similar, but different, temperature-time histories is investigated in Figures 5.3.2.4.5-1 through 3. Additionally, since temperatures (used to develop the parameter) vary with potential repository location (e.g., center and edge), effective thermal conductivities are developed for a variety of different areal mass loadings. Subsequently, ranges of effective thermal conductivity based on areal mass loading are developed to approximate temperature driven variability associated with potential repository edge and center effects (e.g., refer to Figure 5.3.2.4.5-4).

The effective conductivity method of calculating multimode heat transfer is an approximation, and a series of analyses have evaluated its ability to mimic more complex modes of heat transfer. The results of these analyses (Francis 2001 [DIRS 155075]), which are summarized below, indicate that the temperatures calculated by MSTH drift-scale submodels had some sensitivity (up to 2.5°C difference) to effective thermal conductivity at early times. However, beyond 1,000 years after emplacement, the models were insensitive to this parameter.

An effective thermal conductivity used to approximate either thermal radiation or natural convection heat transfer is strongly dependent on temperature. Because the temperature varies in time (Figure 5.3.2.4.5-1), the thermal radiation and natural convection components vary in time. Specifically, the maximum effective thermal conductivity for thermal radiation occurs at the maximum temperature of the heat-generating surface, rather than at the maximum temperature difference between the surfaces. It is a function of the fourth power of the absolute temperatures of the exchanging surfaces as well as surface and geometric radiative properties (e.g., the surface resistance is dependent on the surface emissivity, the geometric resistance is dependent on the view factor). However, the maximum effective thermal conductivity for natural convection occurs at the maximum temperature difference between the surfaces. The temperature of the in-drift components (and how they vary in time) provides the basis for development of effective conductivity.

This part of Section 5.3.2.4.5 focuses on the development of an approximate thermal conductivity to represent thermal radiation. Because some of the analyses studied both radiation and natural convection approximations, some aspects of the natural convection approximation were also discussed. The next part of this section addresses the development of an approximate thermal conductivity to represent natural convection.

5.3.2.4.5.1 Sensitivity of Effective Thermal Conductivity and Resulting Temperatures to Design Details

An illustration of the sensitivity of effective thermal conductivity to the specifics of the design is shown in *Effective Thermal Conductivity for Drift-Scale Models Used in TSPA-SR* (CRWMS M&O 2001 [DIRS 153410], Sections 5 and 6). Analyses conducted for that report compute the effective conductivity for thermal radiation and natural convection using engineered barrier system temperatures and geometry associated with the License Application Design Selection (LADS) Enhanced Design Alternative (EDA) II (CRWMS M&O 1999 [DIRS 107292], Section 5.1). Section 3 of CRWMS M&O (2001 [DIRS 153410]) provides the assumptions associated with the development of the LADS-based parameters. The following are the most important assumptions:

- Heat transfer occurs between concentric cylinders.

- The surfaces are isothermal (i.e., the temperature of a surface does not vary appreciably with respect to angular position).

- The correlation used for natural convection is for an average heat transfer coefficient (CRWMS M&O 2001 [DIRS 153410], Section 5.2) to obtain the correct overall heat flux; however, this method does not capture the variation of temperature due to natural convection air movement patterns.

- The same temperature difference (at any given time) between surfaces is used to generate each component of effective thermal conductivity.

The effective thermal conductivity for thermal radiation, natural convection, and the total (both modes) effective conductivity are shown in Figures 8 through 10 of CRWMS M&O (2001 [DIRS 153410]). These values were calculated using a selected subset (potential repository center) of LADS EDA II temperatures for the waste package, drip shield, and drift wall. In that design, the natural convection component represents about 11 percent of the total heat transfer at the time of peak waste package temperature. At later times, the natural convection component represents about 4 percent of the total. The combined-mode effective thermal conductivity parameter developed in CRWMS M&O (2001 [DIRS 153410], Figure 10) was used in the TH and THC analyses supporting the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]).

Because the design operating temperatures and geometry were somewhat different in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) than in the EDA II, an updated effective thermal conductivity was computed. The temperature (CRWMS M&O 2001 [DIRS 154594]) and geometry (CRWMS M&O 2000 [DIRS 151014]) were calculated for the TSPA-SR design. The differences in the results illustrate the sensitivity of the potential repository drift-scale models to this in-drift parameter. The in-drift temperatures used in the development of the updated parameters were repository-wide averaged values for the waste package, drip shield, and drift wall, using the mean infiltration flux thermal hydrology results obtained from the process model described in the *Multiscale Thermohydrologic Model* (CRWMS M&O 2000 [DIRS 149862]). This provides a better overall representation of the potential temperature variability than the potential repository-center temperatures used in the earlier EDA II analysis.

Figure 5.3.2.4.5-1 shows a comparison between the results for the TSPA-SR design (CRWMS M&O 2000 [DIRS 153246]) and the EDA II results. To about 10,000 years, the EDA II temperatures are greater than the TSPA-SR temperatures, resulting in a larger thermal radiation component and a larger combined-mode effective thermal conductivity parameter. However, the inner (between the waste package and the drip shield) effective thermal conductivity for the TSPA-SR design is larger than it is for the EDA II design, even though at early times the temperatures are lower (at late times the TSPA-SR design temperatures are greater). This is due to differences in drip shield geometry and radiative surface properties (CRWMS M&O 2001 [DIRS 153410], Equation 6). Additionally, the temperature difference between the waste package and drip shield is greater for the TSPA-SR design, resulting in a larger natural convection component.

The sensitivity of the potential repository drift-scale models to the effective thermal conductivity was investigated by applying each of the curves from Figure 5.3.2.4.5-1 to a single LDTH submodel location and comparing the resulting temperature differences at a number of different locations within the EBS. The sensitivity study used a two-dimensional line-source drift-scale thermal-hydrologic submodel (location L4C4), as described in the *Multiscale Thermohydrologic Model* (CRWMS M&O 2000 [DIRS 149862], Section 6). This location was selected because it is near the geographic center of the potential repository footprint and therefore representative of the degree of edge effects for much of the footprint. The submodel applies the active fracture flow model between the fracture and matrix continua in the host rock, as do all the submodels used in this analysis. The submodel calculated the heat flow across the outer air gap (between the drip shield and the drift wall) using a monolithic heat source with the dimensions of the drip shield. The temperature evaluations were made at the upper and lower points of the drip shield and at the crown and springline of the drift wall. Temperature difference evaluations were made for both preclosure and postclosure, as shown in Figures 5.3.2.4.5-2 and 5.3.2.4.5-3, using information from the LADS EDA II design (CRWMS M&O 1999 [DIRS 107292]) and the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]).

Figures 5.3.2.4.5-2 and 5.3.2.4.5-3 show that the heat source temperatures (top and lower drip shield) computed from the TSPA-SR design-based effective thermal conductivity are hotter than those computed using the LADS EDA II design-based conductivity. This is because the effective thermal conductivity outside the drip shield—and, thus, the total effective heat transfer rate across the air gap—is lower, according to Figure 5.3.2.4.5-1. The shift in heat transfer from the air gap to the invert for the TSPA-SR design-based effective thermal conductivity results in lower drift wall temperatures, as indicated in Figures 5.3.2.4.5-2 (preclosure) and 5.3.2.4.1-3 (postclosure). The figures show that a maximum temperature difference between the two cases of about 2.5°C occurs at the waste packages early after closure. After about 1,000 years, the temperature difference is a fraction of a degree at any location considered within the drift.

5.3.2.4.5.2 Comparison of Effective Thermal Conductivity Results to Explicit Radiation Results

Using a two-dimensional LDTH submodel (the L4C3 location, near the center of the potential repository) of the MSTH model (CRWMS M&O 2000 [DIRS 149862]), an explicit representation (using computed view factors) of thermal radiation heat transfer from the drip shield to the drift wall was used to generate temperature time-histories. These temperatures were then used to develop new effective thermal conductivity parameters, based on concentric cylinder correlations for thermal radiation and natural convection. The location of the submodel is in the lower lithophysal host rock unit (tsw35). At this location, the infiltration rate boundary conditions (based on the methodology and input data in CRWMS M&O 2000 [DIRS 149862]) of 6.7 mm/yr for the present-day climate (0 to 600 years), 18.6 mm/yr for the monsoonal climate (600 to 2,000 years), and 27.7 mm/yr for the glacial-transition climate (beyond 2,000 years) (Francis 2001 [DIRS 155075]) are approximately representative of the average infiltration rates over the heated potential repository footprint.

The submodel was exercised with explicit thermal radiation heat transfer and with separate effective thermal conductivities for natural convection and thermal radiation. The results were then used to establish the relative importance of each of the effective thermal conductivity components. Additionally, a determination was made of how well the effective thermal conductivity for thermal radiation actually represents a geometrically complex mode of heat transfer.

Four AMLs were used to develop effective thermal conductivities for the HTOM and LTOM. Sections 5.2 and 5.4 provide a description of how multiple AMLs in drift-scale submodels of the MSTH model are used to evaluate the increasing influence of the potential repository edge as time progresses. The effective thermal conductivity parameters for the HTOM were tested using the base AML of 55 MTU/acre (Table 5.1-1).

As discussed in Section 5.2, the drift-scale submodels normally treat the drift air as a porous medium with a high permeability to capture some of the movement of air due to natural convection. For the effective thermal conductivity comparison, the bulk permeability of the in-drift air was set to zero to eliminate (duplicative) explicit calculation of natural convection. The four two-dimensional TH potential repository drift-scale submodels with explicit thermal radiation represented in the drift were then used to determine the EBS temperatures, and these temperatures were used to develop the effective thermal conductivities for thermal radiation and natural convection. At each given time, the same temperature difference between the drift wall and drip shield was used to develop both parameters. Figure 5.3.2.4.5-4 illustrates the total effective thermal conductivity developed from temperatures averaged from five locations on the heat-generating surface (the drip shield in some of the submodels) and eighteen locations on the drift wall. The total effective thermal conductivity contains a component for thermal radiation as well as natural convection. At early times, the higher AML curves are most appropriate at the central location of the potential repository for this implementation of the submodel. At later times, the most appropriate effective AML for the two-dimensional submodel decreases (based on consideration of three-dimensional mountain-scale effects). The AML-dependent postclosure effective thermal conductivities bound the values obtained from the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) effective conductivity calculation, which are based on temperatures averaged over the potential repository footprint.

To determine the effect of approximating thermal radiation in the emplacement drift using an effective (approximated) thermal conductivity, drip shield and drift wall temperatures were computed using the base AML (55 MTU/acre) for the HTOM and three in-drift heat transfer approaches. The approaches were explicit thermal radiation (with no approximated natural convection), approximated thermal radiation (with no approximated natural convection), and approximated thermal radiation and natural convection. For each approach, the model was run twice to investigate the influence of explicit natural convection in the porous medium used to represent the in-drift air. One run used zero bulk permeability in the air (to suppress explicit natural convection), and the other used a value of 10^{-8} m^2 for air-permeability (the recommended value based on the sensitivity analysis discussed in Section 5.3.2.4.5.3). Although this selected value for the in-drift air bulk permeability is somewhat arbitrary, the sensitivity study conducted for the in-drift air bulk permeability indicates the effective reasonableness of this value within a large range of potential values. However, the "actual" specification of this value will be dependent on a computational fluid dynamics flow solution of turbulent buoyant convection in an open cavity of appropriate geometric scale. Since this information is not presently available, use of the base value (10^{-8} m^2) along with the effective thermal conductivity to estimate the turbulent natural convection in the repository-scale models is recommended based on the results of the sensitivity studies described in this section. Figure 5.3.2.4.5-5 shows the surface-averaged drip shield temperature histories for the six model implementations.

The average drip shield temperatures (Figure 5.3.2.4.5-5), which are based on an effective thermal conductivity parameter for thermal radiation, under-predict the early time temperatures (obtained from explicit thermal radiation) at the drip shield. At closure of the potential repository, the effective thermal conductivity for thermal radiation underpredicts the average surface temperature of the drip shield obtained using explicit thermal radiation by about 10°C. At the time of peak drip shield temperature, the under-prediction is about 6°C. At 1,000 years, the drip shield temperature under-prediction using a combined-mode effective thermal conductivity is about 1°C. The differences between the cases with and without a bulk permeability are slight and occur at early times only. The lowest drip shield temperatures occur when using the combined-mode effective thermal conductivity with a bulk permeability specified. However, this curve is only lower by a fraction of a degree when compared to the temperature time-history curve generated by the combined-mode effective thermal conductivity without a bulk permeability specified for the in-drift elements. The differences between the model results are attributed to conceptual model geometric differences (concentric cylinders compared to eccentric, or off-center, cylinders with an invert).

The drift wall temperatures that correspond to the drip shield temperatures shown in Figure 5.3.2.4.5-5a are much less sensitive to the treatment of heat transfer across the air gap. The drift wall temperatures obtained from the effective thermal conductivity are slightly higher (i.e., have a higher heat transfer rate) than those obtained from explicit thermal radiation. The difference is typically less than a fraction of a degree. Therefore, when host rock temperatures are the driving forces for a process being studied (e.g., drift-scale THC water chemistry and gas-phase compositions at the emplacement drift wall), the choice of an effective thermal conductivity parameter used to represent the in-drift heat transfer processes is adequate. Conversely, when in-drift temperature levels and spatial distributions are the driving forces for a process being studied (e.g., condensation on the coolest surfaces within the drift), explicit representation of thermal radiation is desirable. This conclusion was implemented in the MSTH postclosure calculations in support of the SSPA, as described in Section 5.3.1.3. That is, explicit thermal radiation was used between the drip shield and drift wall in the line-source drift-scale TH submodel, and explicit thermal radiation was also used both under and over the drip shield in the discrete-source drift-scale thermal submodel.

Because the porous media flow codes such as NUFT (V3.0) and TOUGH2 (see Chapters 3 and 4 of this document) are currently incapable of modeling turbulent natural convection in an open-air cavity, the effective thermal conductivity for natural convection within the emplacement drift should be applied. However, since the specification of an in-drift bulk permeability had little influence on temperature predictions, the porous medium approximation in the drift air can be used to simultaneously transport mass across the air gap without introducing any significant error in the temperature distribution. It is reasonable to specify a bulk permeability to the in-drift air elements of at least a value equal to the fracture permeability in the host rock.

The applicable curves for effective thermal conductivity for natural convection are shown later in this section. A detailed analysis for the selection of a proper in-drift bulk permeability also follows.

5.3.2.4.5.3 The Effect of the Bulk Permeability of In-Drift Air on Temperature Distributions Calculated by the Line-Source Drift-Scale Thermal-Hydrologic Submodel

The LDTH submodel of the MSTH model (CRWMS M&O 2000 [DIRS 149862]) uses a porous medium to model the in-drift air and uses an approximated thermal conductivity that includes heat transferred by natural convection between concentric cylinders. The previous part of this section considered bulk permeabilities of either $0\ m^2$ or $10^{-8}\ m^2$ assigned to the in-drift air elements. In those simulations, it was found that for either an explicit thermal radiation or an effective thermal conductivity (representing thermal radiation and natural convection), the influence of the in-drift bulk permeability on the temperature at the drip shield or drift wall was negligible. In this part of the section, a more comprehensive range of bulk permeabilities is considered, along with hydrologic and temperature results.

The model selected for the sensitivity analysis of the HTOM is a two-dimensional LDTH submodel from the MSTH model. The submodel considered was at the base AML (55 MTU/acre). The submodel location (L5C3; see Section 5.3.1.2) was selected because it is near the L4C4 and L4C3 locations and because it is not near the top of the lower lithophysal subunit. The surface infiltration rates at this location (based on the methodology and input data in CRWMS M&O (2000 [DIRS 149862]) are 5.7 mm/yr for the present-day climate (0 to 600 years), 15.1 mm/yr for the monsoonal climate (600 to 2,000 years), and 23.2 mm/yr for the glacial-transition climate (beyond 2,000 years) (Francis 2001 [DIRS 155075]). It includes explicit thermal radiation for the in-drift elements, and it applies the effective thermal conductivity curve for natural convection heat transfer. Table 5.3.2.4.5-1 gives the range of bulk permeability for the air elements in the emplacement drift considered in this sensitivity study. The locations and TH parameters used to evaluate differences in the models are the:

- Drift wall crown (temperature and liquid saturation)
- Drift wall springline (temperature and liquid saturation)
- Top of the drip shield (temperature and relative humidity)
- Base of the drip shield (temperature and relative humidity)
- Bottom-center of the invert (temperature and liquid saturation).

These locations illustrate the potential for both vertical and horizontal variability associated with the in-drift bulk permeability specification.

Temperature Dependence on In-Drift Bulk Permeability–Figures 5.3.2.4.5-6 through 5.3.2.4.5-8 show the temperatures at the base of the drip shield, at the crown of the drift wall, and at the bottom-center of the invert for the range of in-drift bulk permeabilities described in Table 5.3.2.4.5-1.

Figure 5.3.2.4.5-6 shows the temperature histories at the base of the drip shield for the range of air permeabilities; the temperatures at the top of the drip shield showed even less sensitivity to air-permeability. It is evident from Figure 5.3.2.4.5-6 that the in-drift bulk permeability does not affect the drip shield temperature for most of the permeability values, and permeability has only a small effect (less than 4°C) for the largest value investigated ($2\times10^{-5}\ m^2$). For the high bulk permeability case, the drip shield temperatures are somewhat lower from closure of the potential repository until about 200 to 300 years. The reduction in temperature at the drip shield surface is reasonable, since the higher air-permeability results in a larger rate of heat transfer from the heat source to the drift wall. However, the computational burden of the high air-permeability was significant; this case could not be run to the full 10^6 years due to a continuous reduction in time step. The simulation reached about 3,000 years and was manually terminated because the time step had decreased to only a fraction of a second. Time step reductions occurred in the simulation due to the disparity in fluid velocities associated with the air elements inside the drift and the adjacent host rock elements.

Since the porous media flow codes describe physical processes, this apparent numerical "problem" is actually an indication of the importance of turbulent natural convection within the emplacement drift. That is, even though the temperature difference between the drip shield and the drift wall is small at late times, the length scales associated with these components (e.g., the drift wall) still ensures a highly turbulent flow condition (e.g., the fluid Rayleigh number is still very large at late times) around the interior (drip shield) and exterior (drift) walls. (Note: the fluid Rayleigh number is based on appropriate fluid properties, a length scale, and a temperature difference such that it provides an indication of turbulent or laminar flow within the drift.) An in-drift bulk permeability can be defined based on knowledge of the fluid Rayleigh number. As shown in Webb and Hickox (2001 [DIRS 154777]), a Rayleigh-number-based effective permeability for the in-drift air elements increases as the fluid Rayleigh number to the one-half power. Therefore, for large Rayleigh numbers, the required effective permeability for in-drift flow becomes very large. As indicated above, large values of air-permeability pose problems for the porous media flow codes. Indeed, this is the primary motivation for the development of an effective thermal conductivity for turbulent natural convection (heat transfer only) used in the porous media flow code coupled with a (nonzero) value for the in-drift air-permeability to ensure mass transfer within the drifts (see the next subsection).

Figure 5.3.2.4.5-7 shows that the temperature histories at the drift wall crown are also insensitive to the air-permeability range investigated. The temperatures at the springline of the drift wall are even less sensitive than at the crown. The highest value of air-permeability slightly shifts the distribution of heat flow, increasing the fraction toward the drift wall (and increasing the drift wall temperature), while decreasing the fraction through the invert (and decreasing the invert temperature). However, the magnitude of the shift in heat transfer results in a temperature change of only a few degrees at those locations.

Effect of In-Drift Bulk Permeability on Hydrologic Parameters–Figures 5.3.2.4.5-9 through 5.3.2.4.5-12 show the time histories of the relative humidity and air-mass fraction at the base of the drip shield and of the saturation in the near-field rock at the drift wall and in the invert. These hydrologic parameters were calculated for the range of in-drift bulk permeabilities described in Table 5.3.2.4.5-1.

The relative humidity histories illustrated in Figure 5.3.2.4.5-9 are directly related to the corresponding temperature histories in Figures 5.3.2.4.5-6. The relative humidity histories for the base case and "fracture k_b" air permeabilities are nearly identical due to the nearly identical temperature time-histories and approximately similar in-drift permeabilities. In contrast, the high air-permeability case produced a slightly higher relative humidity than the base case. This is due to a combination of slightly lower temperatures and higher in-drift permeability, allowing more water vapor to enter the emplacement drift from the surrounding host rock. As more water vapor enters the drift, the air mass fraction in the drift elements decreases, increasing the numerator of the fraction that defines relative humidity (water-vapor pressure divided by water-vapor-saturation pressure at the local temperature). Figure 5.3.2.4.5-10 shows that the in-drift air mass fraction for the high bulk permeability case is generally lower than the base case for the first 1,600 years, which is the major cause of the slightly higher relative humidity for this case.

For the low air-permeability case, the prohibition of vapor flow from the near-field rock forces a constant air mass fraction. However, the saturation pressure, which is the denominator of the fraction that defines relative humidity, increases with temperature, resulting in a depressed relative humidity during the period of high temperature.

Figure 5.3.2.4.5-11 shows the negligible sensitivity of the saturation histories at the drift wall crown to the range of air permeabilities investigated. The histories at the drift wall springline show even less sensitivity to the air-permeability. Figure 5.3.2.4.5-12 shows that the sensitivity of the invert saturation to in-drift air-permeability is also weak. Slight differences occurred between the four air-permeability cases because of differences in mass transfer rates at the drift wall contacts, both at dryout and later at resaturation. The base case invert saturation also showed some numerical instability during rewetting; similar numerical artifacts were observed in the invert thermal conductivity sensitivity calculations described in Section 5.3.1.4.10.

Based on temperature and hydrologic parameter results, it is concluded that the potential repository drift-scale models are insensitive to the choice of bulk permeability specified for the in-drift air elements. A nonzero bulk permeability must be assigned to the in-drift elements to avoid artificial depression of relative humidity during the high temperature period (Figure 5.3.2.4.5-9), and all three of the nonzero values investigated produced similar temperature and hydrologic results. The higher end of the permeability range investigated results in more realistic movement of air; however, it also greatly increases computational run times. The intermediate values (base case and fracture bulk permeability) of air-permeability allow some movement of air and produce realistic values of relative humidity without the long computational times associated with a high air-permeability.

Thus, the development of an effective thermal conductivity for natural convection heat transfer has succeeded in that it produces realistic temperatures and hydrologic parameters without long computational time requirements. It reduces the complex mode of heat transfer to a faster, simpler computational model, with the only loss of information being the small variations of temperature on the drip shield surface and on the drift wall surface.

Sensitivity Studies of a High Bulk Permeability Inside the Drift Without the Effective Thermal Conductivity–The high air-permeability case from Table 5.3.2.4.5-1 was rerun without including the effective thermal conductivity for turbulent natural convection using the same LDTH submodel of MSTH model (CRWMS M&O 2000 [DIRS 149862]). The result was compared to the low air-permeability case described above; the low permeability case included an effective thermal conductivity for natural convection while specifying a bulk permeability of zero in the drift. This comparison provides an estimate of how well a porous medium model using a large in-drift air-permeability represents heat transfer driven by (turbulent) buoyancy effects between the drip shield and the drift wall. The effective thermal conductivity (averaged over the hot and cold surfaces) for buoyant, turbulent natural convection is based on an empirical correlation for concentric cylinders. This correlation has been tested against experimental data and Navier-Stokes computational fluid dynamics (CFD) numerical models. For the purposes of the comparison described below, the effective thermal conductivity model with zero air-permeability is expected to give more physically reasonable temperature predictions than the porous medium code using a high permeability. Because of the zero air-permeability, relative humidity predictions would not be more physically realistic.

Figure 5.3.2.4.5-13 shows the temperature histories at the top of the drip shield for the two cases. The histories at the base of the drip shield are almost identical, but show slightly less sensitivity. The high air-permeability case without an effective thermal conductivity for natural convection underpredicts the heat transfer rate from the drip shield to the drift wall (i.e., the drip shield temperature is higher than the effective thermal conductivity case with zero air-permeability).

Figure 5.3.2.4.5-13 can be compared with Figure 5.3.2.4.5-6, which compares the drip shield temperature using the porous medium model with an additional effective thermal conductivity for natural convection. When a high air-permeability is combined with an effective thermal conductivity, as in the lowest temperature case from Figure 5.3.2.4.5-6, the calculation takes credit for natural convection in two ways, resulting in a somewhat low peak drip shield temperature. However, the use of a high air-permeability in a porous medium model, with no effective thermal conductivity for natural convection, does not adequately capture the extent of heat transfer from natural convection, resulting in a somewhat high peak drip shield temperature. It should be noted that the differences in peak drip shield temperature are relatively small (±4°C) compared to the total amount of heating of the drip shield (135°C) above ambient temperature.

Figure 5.3.2.4.5-14 shows the temperature at the crown of the emplacement drift. The early time temperatures are slightly lower (about 1°C) for the case of high air-permeability and no effective thermal conductivity for natural convection. This is due to a slight shift of heat flow to the invert to compensate for the underprediction of convective heat transfer.

The conclusion of this comparison is that, for reasonable computation times, in-drift air-permeability in a porous medium model cannot be made large enough to reproduce the temperature characteristics associated with the effective thermal conductivity for turbulent natural convection.

5.3.2.4.5.4 Comparison of Turbulent Natural Convection Air Flow in a Porous Medium Model and a Navier-Stokes Computational Fluid Dynamics Model

The correlation-based approach described above is based on concentric cylinder geometry. There are also some empirical correlations available for eccentric cylinders in which the center of the inner cylinder is offset (vertically downward in the current design). However, the noncircular nature of the drip shield and the presence of the invert limit the benefit of extending an approach based on published correlations to eccentric cylinders. An alternative approach is to calculate the velocities and temperature distributions for natural convection between the drip shield and drift wall (and between the waste package and drip shield) using Navier-Stokes CFD models. The advantage of such calculations is that the geometric details can be accurately modeled. The results of the calculations can be used to develop design-specific correlations for the LDTH and (DDT) submodels.

Preliminary results of the CFD analyses can be used to assess the applicability of the porous medium model with supplemental concentric cylinder correlations for natural convection, which was employed to calculate temperatures and humidities for the SSPA Volume 2 (McNeish 2001 [DIRS 155023]) TSPA.

Webb and Hickox (2001 [DIRS 154777]) used a finite element CFD (FIDAP V8.0) code to analyze natural convection in an open space using the Navier-Stokes equations and in a porous medium using correlation-based Nusselt numbers for the heat transfer between the moving air and each cylinder. The resulting temperature, vertical velocity, and heat flux distributions for the two methods are shown in Figures 5.3.2.4.5-15 through 5.3.2.4.5-17. These figures represent the results using nondimensional numbers. The figures normalize distance by dividing by the inner cylinder radius. Thus, for the temperature and velocity figures, zero is at the inner cylinder and 2.6 is at the outer cylinder. The heat flux figure measures normalized distance around the outer cylinder perimeter, with zero at the bottom and 2.6 is at the top. Temperature was normalized by first subtracting the average of the two wall temperatures, then dividing by the difference between the wall temperatures. Thus, zero on the normalized temperature scale is the average temperature of the walls. Velocity was normalized by dividing by the square root of the product of the gravitational constant, thermal expansion coefficient of air, difference between the wall temperatures, and radial distance between the walls. Heat flux was normalized by dividing by the product of the diameter of the outer cylinder, the air thermal conductivity, and the difference between the local wall temperature and average air temperature.

Figures 5.3.2.4.5-15 through 5.3.2.4.5-17 show that the porous medium approach can produce reasonable average values, but that the details of the spatial distributions are not replicated by the porous medium model. The computational times for the CFD model were not excessive in this case (minutes) because the model was run in a steady-state mode. Transient calculations would use significantly more computational resources (days of computational time for convergence to steady-state for this short-transient problem) and would only be justifiable to develop correlations for use in more computationally efficient models, such as the MSTH model.

Natural convection has also been calculated using the Navier-Stokes CFD capability of ANSYS (BSC 2001 [DIRS 155024]). The initial results were a successful comparison of calculated temperatures and velocities for a concentric cylinder geometry to an empirical correlation from the literature. Initial calculations for a realistic geometry that includes both the invert and drip shield are shown in Figure 5.3.2.4.5-18. This calculation used a steady-state solver with a 1 kW waste package (about 0.2 kW/m) and a 40°C boundary condition 5 m into the near-field rock. This heat source is consistent with a pressurized water reactor waste package several centuries after the thermal peak. In the calculation, the drift wall temperature was about 55°C and the waste package temperature was about 62°C. Peak velocities in this calculation are in the range of 10 to 15 cm/s.

The quarter-scale ventilation test was also used to simulate natural convection by ceasing forced convection and allowing the thermal profile to stabilize, using a heat flux of 0.12 kW/m and an ambient temperature boundary condition at the edge of the insulation (Jurani 2001

[DIRS 155128]). The heat flux was equivalent to a full-scale heat load of about 0.5 kW/m, similar to a boiling water reactor waste package about a century after emplacement. However, the boundary temperature was lower than for a potential repository situation, resulting in lower-than-repository temperatures at the drift wall and waste package. The test was modeled with the Fluent V5.5 software package. The air velocity profile is shown in Figure 5.3.2-1. The peak velocities of 10 to 16 cm/s are consistent with those in the waste package design initial calculation.

5.3.2.4.5.5 Summary

Based on the results described in this section, the MSTH model used for the SSPA Volume 2 (McNeish 2001 [DIRS 155023]) TSPA used explicit thermal radiation, an effective thermal conductivity for turbulent natural convection, and in-drift air bulk permeability of 10^{-8} m^2.

Figures 5.3.2.4.5-19 and 5.3.2.4.5-20 show the effective thermal conductivities for natural convection that were used, based on this section, in the base case evaluations of the HTOM and LTOM of the design evaluated for the SSPA. In developing these effective conductivities, the three-dimensional effect of the potential repository edge was represented by considering multiple AMLs within the centrally-located two-dimensional LDTH submodel. A lower AML in the two-dimensional submodel is implemented by using a larger effective drift spacing, which in turn reduces the drift wall temperature. At lower drift wall temperatures, radiation is less effective, and the drip shield (and waste package) temperatures must increase to transfer the heat. Thus, the temperature difference between the surfaces is greater for the lower AML and the effective thermal conductivity for natural convection is larger because buoyant convection is driven by the temperature difference.

The effective thermal conductivity for turbulent natural convection based on a correlation developed for concentric cylinders probably does not introduce significant uncertainty in EBS component temperatures (more than several degrees centigrade) based on the insensitivity of those temperatures (Figures 5.3.2.4.5-5, 5.3.2.4.5-6, and 5.3.2.4.5-13). The effective thermal conductivity for natural convection is more sensitive to the temperatures at which the correlation is evaluated (Figure 5.3.2.4.5-1). Efforts to update the effective conductivity for the current design values (rather than using an effective conductivity developed for an earlier design) have proved worthwhile.

In general, a nonzero bulk permeability in the emplacement drift should be specified to reasonably compute the moisture effects on the in-drift relative humidity. The base case in-drift bulk permeability (10^{-8} m^2), in conjunction with the effective thermal conductivity for natural convection, provides nearly the same EBS temperature results while allowing for an appropriate representation of the heat and mass transfer processes occurring within the emplacement drifts. However, if only near-field (rather than EBS) processes are required of a model, a value of zero for air-permeability in the drift is adequate.

5.3.2.4.6 The Influence of Axial and Cross-Sectional Variations in Temperature on In-Drift Condensation

The variations in geometry and thermal output of waste package will result in variation of temperature within a cross-section of an emplacement drift and along the drift axis. Because the in-drift air will be circulated due to natural convection, resulting in a spatially uniform composition, water will preferentially evaporate from warmer surfaces and condense on cooler surfaces due to the small difference in equilibrium of vapor pressure at the temperatures of the surfaces. Surface roughness and the presence of dust will influence the vapor pressure at the surfaces.

The MSTH model (CRWMS M&O 2000 [DIRS 149862]) includes evaporation and condensation on in-drift surfaces, based on thermodynamic properties of the gas and liquid phases. The water then moves along the drift surface under the influence of gravity and capillary forces in the highly permeable porous medium used to simulate the air (air properties are discussed in Section 5.3.2.4.5). This treatment captures much of the two-phase process; however, it does not calculate the details of the geometry of condensation (film thickness or growth of individual drops) on surfaces which can be affected by roughness and on dust which can dissolve into the condensing water.

The TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) model includes humid-air corrosion of the waste packages and drip shields when in-drift air humidity is high enough to deliquesce onto salts in the dust. Therefore, condensation on the waste packages and drip shields is assumed in the current implementation of corrosion in TSPA. In TSPA-SR (CRWMS M&O 2000 [DIRS 153246]), radionuclide transport in the engineered barrier system was assumed to be diffusive until breach of the drip shields by corrosion or disruptive events; the basis of this assumption was that condensate film or drops could be too thin (or small) to flow, flow very slowly, or be hindered by corrosion products, detrital material, or mineral precipitates.

For one SSPA Volume 2 (McNeish 2001 [DIRS 155023]) unquantified uncertainty sensitivity study, the condensation model was improved (Section 8.3.2). Condensation on the underside of the drip shield can occur in the improved model if the vapor pressure at the invert is higher than the saturation pressure at the drip shield. This situation is implemented by assuming there is condensation when the drip shield temperature is less than the invert temperature; the implementation ignores chemical and capillary effects on the vapor pressure in the invert. Condensation is assumed to drip from the drip shield onto the waste package, analogous to the dripping of seepage from a drip shield breach. The volume of condensation is sampled from zero to 100 percent of the evaporation rate of water from the invert (an output of the MSTH model). This sampling qualitatively accounts for the competition for evaporated water by other cool surfaces such as the drift wall and for run-off of some of the condensate along the side of the drip shield.

Improvements in the three-dimensional DDT submodel of the MSTH model have increased the accuracy of in-drift temperature history calculations (Sections 5.3.1 and 5.3.2) that support the improved condensation model described in Section 8.3.2. Results of the base case calculations (Buscheck 2001 [DIRS 155243]) for the HTOM and LTOM are summarized in

Tables 5.3.2.4.6-1 and 5.3.2.4.6-2, respectively. Those results are the focus of the discussion following the tables.

In addition to being an input to the improved, but simple, condensation model in Section 8.3.2, the in-drift temperature histories could be used in detailed condensate geometry calculations in support of a potential license application. Section 10.3 includes a discussion of models to determine condensation film thickness as a function of substrate material, temperature, and relative humidity, to estimate the area for diffusion of radionuclides within the film. That analysis could be useful in developing a model to determine if condensation could form a source for slow flow that could support advection. Test results from the quarter-scale canister tests (Howard et al. 2001 [DIRS 153282]) and from the scope of work that is identified in the technical work plan for the sealed section of the ECRB cross-drift (BSC 2001 [DIRS 155051], Section 1, Items 27 to 33) are other inputs that can be used to support condensate formation and flow modeling.

Table 5.3.2.4.6-1 illustrates the temperatures in three cross-sections through the ten waste package computational cell for the HTOM. The cell includes eight full waste packages and two half waste packages, with the distribution of waste package types and thermal powers being representative of the full inventory of the potential repository. The three cross-sections are through the mid-lengths of the hottest waste package (pressurized water reactor, PWR), an average power waste package (boiling water reactor, BWR), and a cool waste package (defense high level waste DHLW). The times selected include the time of peak preclosure temperature, just after closure, peak postclosure temperature, three times during the slow cooling of the potential repository (as the waste decays), and a final time at which near-ambient temperatures have been reached. The DDT submodel represents radiation under and above the drip shield explicitly, but uses a perimeter-averaged correlation to represent natural convection. More accurate temperatures along the drift wall perimeter will be available when Navier-Stokes computational fluid dynamics models are applied to this system. Section 5.3.2.4.5 illustrates initial results of such models.

During the preclosure period, the low relative humidity of the ventilation air will limit the water content of the in-drift air enough that water films will be negligible. At the peak of the postclosure temperature for the HTOM, all temperatures are sufficiently high that water films would not form. However, under some conditions, highly deliquescent salts in dust on some components may cause condensate formation at low humidity or elevated temperature; these conditions are being studied in support of a potential license application.

Two thousand years after the waste emplacement, before temperatures have cooled to below-boiling values, the range of temperature differences on all surfaces within the three-dimensional cell is less than 4°C. Within a cross section, the range is as little as several tenths of a degree at the cool waste package to as much as almost 3°C at the design basis (hottest) waste package. Along the drift axis, the range is less than 1°C at the drift wall, and as much as about 3°C at the waste package. Thus, the axial range is similar to the range within a cross section.

As temperatures decrease through the boiling point, the coolest surfaces in the drift are at the drift wall. The invert zone under the drip shield is slightly warmer than the drip shield itself.

Since the invert temperature is an average through its half-depth, its surface is hotter than either its average or the drip shield surface. Thus, for the natural convection (perimeter-averaged) correlation and the low value of invert thermal conductivity used in the calculation, condensation would be favored on the drift wall near the coolest waste package. However, condensation depends on surface conditions as well as temperature; thus the temperature relationships are not enough to draw conclusions about condensate geometry on rock, titanium, and gravel.

Airflow patterns of natural convection are expected to shift the temperature of the drip shield (upper region) upward and the temperature of the invert surface under the drip shield downward. Therefore, natural convection could result in a cooler invert than the drip shield, reducing potential condensation on the underside of the drip shield. As corroboration of this logic, observations of the quarter-scale canister test were that the invert was cooler than the drip shield, with no dripping or rivulets observed under the drip shield (Howard et al. 2001 [DIRS 153282]).

Table 5.3.2.4.6-2 illustrates the temperatures in five cross-sections through the ten waste package computational cell for the LTOM. The cell includes the same sequence of waste packages as for the HTOM. However, there are variable length gaps between the waste packages with the goal of smoothing the local lineal heat loading. This geometric smoothing is an alternative to the axial radiation heat transfer between waste package ends that smoothes the local lineal heat loading in the HTOM. The five cross-sections are through the mid-lengths of the hottest waste package (PWR), an average power waste package (BWR), a cool waste package (DHLW), a warm gap, and a cool gap between waste packages. The times selected include the time of peak preclosure temperature, just after closure, three times representing the broad period of near-peak postclosure temperature, during the slow cooling of the potential repository (as the waste decays), and a final time at which near-ambient temperatures have been reached.

During the preclosure period, the low relative humidity of the ventilation air will limit the water content of the in-drift air enough that water films will be negligible. Under some conditions, highly deliquescent salts in dust on some components may be able to cause condensation at low humidity; these conditions are being studied in support of a potential license application. As soon as ventilation ceases for the LTOM, all temperatures are sufficiently low that condensate could form.

At the time of peak waste package temperature, the range of temperature differences on all surfaces within the three-dimensional cell is about 10°C. Within a cross section, the range is as little as 1°C at the cool waste package to as much as 8°C at the design basis (hottest) waste package. Along the drift axis, the range is about 2°C at the drift wall, and about 9°C at the waste package. Thus, the axial range is similar to the range within a cross section.

As temperatures cool, the coolest surfaces in the drift are at the drift wall. The invert zone under the drip shield is slightly warmer than the drip shield itself. Because the invert temperature is an average through its half-depth, the surface is hotter than either the average or the drip shield surface. As for the HTOM, shifts in temperature patterns around the perimeter of air flow loops could reverse the temperature relationship between the drip shield and invert surface, resulting in little condensation on the drip shield underside.

Summary–Temperatures and invert evaporation rates are used as inputs to the drip shield condensation model (see Section 8.3.2) for one SSPA Volume 2 (McNeish 2001 [DIRS 155023]) unquantified uncertainty sensitivity study. Current values of the three-dimensional temperature distribution from the MSTH model would produce condensation on the underside of the drip shields for that model.

The distribution of temperatures within the drift (and the surface properties of the drift wall, drip shield, and invert gravel) will determine the location and thickness of condensation films. Natural convection effects on the temperature distribution along the drip shield perimeter (not included in the MSTH model results) could result in a cooler invert than the drip shield, reducing condensation on the underside of the drip shield. This uncertainty (the absence or presence of condensation under the drip shield) will be addressed in more sophisticated models, the quarter-scale test, and the 44 percent-scale tests in support of a potential license application.

5.3.3 Quantification of Uncertainty Using Analogues

Analogues and multiple lines of evidence from several other sections of this document are pertinent to the in-drift thermal-hydrologic processes within the EBS. In Section 3.3.2, Infiltration Model, there is discussion on the infiltration analogues that have been done. These are pertinent to the in-drift thermal-hydrologic processes in that the analogue is corroborating the amount of infiltration that is being predicted and the resulting seepage that potentially make its way through the various geologic components to the potential repository level. Section 3.3.3, Flow in PTn, discusses the flow potential in the PTn and TSw units. These analogues are useful in understanding lateral flow in the units.

As stated in Section 3.3.4.7, natural analogue studies of fluid flow processes for similar geologic and hydrologic settings provide multiple lines of evidence. Studies have been ongoing at various locations on the Nevada Test Site. One area of similar geologic and hydrologic settings is Rainier Mesa (see Section 3.3.4.7). Another area under investigation is Yucca Mountain. Section 3.3.6.5 discusses some of the "self-analogues" that have been ongoing at Yucca Mountain. Of particular interest are the analogues of geothermal systems and how the coupled processes that are being modeled relate to them (see Sections 3.3.6.5 and 3.3.7.6).

In Section 4, Seepage, there are analogues identified that discuss other scientific work regarding the flow of water in underground openings. Of particular relevance are the discussions in Sections 4.3.1.7, 4.3.2.7, 4.3.5.7, 4.3.6.7, and 4.3.7.7.

Further discussions on natural analogues are contained in the S&ER (DOE 2001 [DIRS 153849], Section 4.2.2.2.3.3). The analogues identified in that report and the aforementioned discussion can be used to demonstrate that the effects of decay heat on waste movement can be evaluated. They also serve to aid in the development and understanding of the process models and abstractions, and predicting future conditions. There is a wide range of information available, from core-scale and outcrop evaluations of fossil thermal-hydrologic-chemical couple processes, understanding of efficient heat transfer mechanism, changes in operating geothermal fields, to dynamic processes with mechanical changes.

5.4 SUMMARY AND PARAMETERS PROVIDED TO TOTAL SYSTEM PERFORMANCE ASSESSMENT

This section summarizes the results of Section 5. Sections 5.3.1.3 and 5.3.2.3 describe changes made to the MSTH model to implement improvements developed since the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]). Sections 5.4.1 and 5.4.2 present results using the improved MSTH model to calculate in-drift thermal-hydrologic conditions for the HTOM and the LTOM, respectively. Section 5.4.3 summarizes the results of applying the MSTH model, its submodels, or other models to investigate the sensitivity of in-drift thermal-hydrologic performance to uncertainties and parameters.

Section 5.2 describes the implementation of the MSTH model (CRWMS M&O 2000 [DIRS 149862]) in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]). The remainder of the section describes the current implementation of the MSTH model. The most straightforward way to calculate the in-drift thermal-hydrologic parameter histories would be to set up the entire mountain in the MSTH model, including heat and mass transfer at all locations, three-dimensional geometric aspects, and finer zone size in regions of highest gradients and regions important to performance. Unfortunately, such a model would run slowly, perhaps with the simulation time clock running slower than real time. To decrease computational time and memory demands, a common practice is to use nested grids. In this approach, the initial problem is set up with coarse gridding over the full domain. The problem is then rerun repeatedly with smaller and smaller domains and finer zone sizes. Thus, each iteration uses the results from the previous iteration as the input boundary conditions.

In the MSTH model, this idea is developed further. In addition to geometric nesting, the MSTH approach also includes dimensionality nesting (combining two- and three-dimensional results) and physics nesting (combining conduction-dominated results with heat and mass transfer results). Table 5.4-1 provides a roadmap of the submodels and the sequential steps used to combine their outputs. The result is a set of thermal-hydrologic parameter histories (subsystem performance measures) that incorporate the overall footprint of the potential repository, the stratigraphy and infiltration flux distribution, the location of potential individual repository drifts, and the arrangement of individual waste packages (with individual thermal power output histories) within the drifts. The model includes radiation, convection, and conduction heat transfer modes; the movement of liquid and gaseous fluids; and phase change effects.

The thirteen-step process is illustrated in Figure 5.2-2. The SMT, SDT, and LDTH submodels are combined (as described in Steps 1 to 7) to produce the LMTH combined temperatures. Then, the LMTH and DDT submodels are combined (as described in Steps 8-11) to produce the DMTH combined temperatures. Finally, the LDTH submodels are used with the DMTH temperatures to develop the values for all other parameters output by the model.

The thirteen-step process is one of a number of possible computationally efficient methods of combining submodels to address dimensionality, physical processes, and geometric complexity. The method has evolved with the TSPA system-level model. This evolution is based on assumptions or separate calculations that conclude neglect of some processes at some scales will not significantly affect the thermal-hydrologic performance measures. For example, three processes that could have been included in the MSTH model, but were not, are east-west convective loops above the drifts, north-south convective loops wider than the half-drift spacing, and axial movement of air and water vapor within the drift. Each of these effects could be calculated with the submodels and implemented in the full MSTH model if found to be significant. Similarly, if results of thermal-hydrologic-chemical or thermal-hydrologic-mechanical calculations indicate changes in hydrologic parameters over time, these changes can be included in future implementations of the MSTH model. It is expected that the MSTH model implemented for a potential license application would include additional capabilities such as those listed in this paragraph.

5.4.1 Higher-Temperature Operating Mode Base Case Results

This section describes the MSTH model base-case calculations (Buscheck 2001 [DIRS 155243]) for the HTOM, which includes the mean, upper, and lower infiltration-flux scenarios. Figure 5.4.1-1 is a plan view of the MSTH model representation of the potential HTOM repository; also shown are the geographic locations for which TH conditions are shown in Figures 5.4.1-2 and 5.4.1-3. These locations were chosen to illustrate the manner in which TH behavior is influenced by proximity to the edges of the potential repository. Three of these locations are close to the center of the potential repository; two are located in the extreme northeast and southwest corners of the potential repository area, and two are at the extreme eastern and western edges of the potential repository, approximately midway between the northern and southern boundaries of the potential repository. The temperature and relative-humidity histories fall into three distinct clusters: one for the potential repository center, one for the potential repository corners, and one for the potential repository edge locations (Figure 5.4.1-2). In addition, the relative humidity reduction can be classified into three sequential periods (Figure 5.4.1-2).

During an early period which lasts from 200 to 1,000 yr (Figures 5.4.1-2c and 5.4.1-3a), the relative humidity reduction on waste packages depends on the magnitude and duration of rock dryout. The duration of rock-dryout increases with distance from the potential repository edges. The farther a given waste package is located from the potential repository edge, the longer the duration of boiling in the local host rock and the longer the duration of rock dryout (and relative humidity reduction). The surface of the waste packages always have a lower relative humidity than the adjacent host rock; consequently, during the early period, the reduction in relative humidity on waste packages increases with distance from the potential repository edges.

The depth of dryout varies with location within the footprint and with infiltration flux. The deepest horizontal extent of boiling temperatures was 13.1, 10.6, and 10.1 m from the drift center, for the lower, mean, and upper infiltration flux scenarios, respectively.

An intermediate period, which lasts from 1,000 yr to about 20,000 yr, during which time heat-transfer in the drift controls the magnitude of relative humidity reduction on waste packages. During this period, the reduction in relative humidity on waste packages decreases with distance from the potential repository edges, which is the reverse of the trend during the early period. During the intermediate period, the reduction in relative humidity is greater at the potential repository edges because the efficiency of thermal radiative heat transfer decreases with temperature. Consequently, for a given local heat generation rate there is a larger temperature difference $\Delta T_{\text{wp-dw}}$ between the waste package and drift wall at locations with lower temperature (such as occurs close to the potential repository edges). Moreover, the reduction in relative humidity, which depends on the ratio of $P_{sat}(T_{dw})/P_{sat}(T_{wp})$, results in a larger relative humidity reduction for a given $\Delta T_{wp\text{-}dw}$, where P_{sat} is the saturation vapor pressure, T_{dw} is the drift wall temperature, and T_{wp} is the waste package temperature.

A late period, beginning around 20,000 yr, during which time the reduction in relative humidity on waste packages becomes decreasingly sensitive to proximity to the potential repository edges. For a given waste package type, the reduction in relative humidity becomes increasingly similar across the potential repository area.

Figure 5.4.1-4 shows the influence of the edge-cooling effect. Locations close to the potential repository edges cooling more quickly than those at the center. Figure 5.4.1-5 shows the development of the reduction in relative humidity on waste packages. At early times, the reduction in relative humidity increases with distance away from the potential repository edges, while at intermediate to later times, the reduction in relative humidity decreases with distance from the potential repository edges.

Figures 5.4.1-3b and 5.4.1-3c show the relationship between liquid saturation in the invert and evaporation rate. During early times, while the invert is dry, the evaporation rate is zero. The onset of rewetting in the invert corresponds to the end of the boiling/rock-dryout period. Consequently, the time of the onset of rewetting increases with distance from the potential repository edges. The two geographic locations that experience a larger eventual increase in liquid saturation in the invert correspond to the two locations wherein the local host rock is either the middle or the lower nonlithophysal Topopah Spring welded tuff unit (Tptpmn or Tptpln). Wherever the local host-rock unit is comprised of the lower lithophysal unit (Tptpll), the maximum liquid saturation in the invert is nearly the same (and lower than in locations where the local host-rock unit is either Tptpmn or Tptpln). Apparently, there is a difference in rewetting behavior in the invert that depends on the local host-rock unit. The second spike in the invert evaporation rate occurs shortly after 600 years when a substantial increase in infiltration flux occurs. The increase in infiltration rate is accompanied by an increase in liquid-phase flux into the invert, which makes more water available for evaporation in the invert.

Figure 5.4.1-6 shows the complementary cumulative distribution functions for temperature and relative humidity on the drift wall and on the waste package for the mean, lower, and upper infiltration-flux scenarios. For the mean-infiltration-flux scenario, the peak waste package temperature ranges from 126.1° to 184.9°C. The peak waste package temperature is similar for the mean and lower infiltration-flux scenarios. The upper infiltration-flux scenarios result in lower peak waste package temperatures, particularly for the coolest waste packages; the range for this scenario is 105.4° to 183.1°C. The time required for the drift-wall to cool down to 96°C (which is the boiling point of water at the potential repository horizon) is more sensitive to infiltration flux than peak temperature (Figure 5.4.1-6b). The time required for the waste package to attain relative humidity equal to 80 percent is similar for the mean and upper-infiltration flux scenarios (Figure 5.4.1-6c). The lower-infiltration-flux scenario results in much more persistent relative humidity reduction on waste packages, particularly for the driest waste packages. The waste package temperature at the time when relative humidity equals 80 percent on the waste package is similar for the mean and upper infiltration-flux scenarios

(Figure 5.4.1-6d); the lower infiltration-flux scenario results in lower temperatures when relative humidity equals 80 percent is attained.

Figure 5.4.1-7 shows the waste package-to-waste package variability of temperature and relative humidity at a location in the potential repository relatively close to the geographic center for the mean infiltration-flux scenario. Peak waste package temperatures range from 152.3° to 180.1°C. The use of line-load waste package spacing results in a relatively narrow range of peak temperatures (27.8°C). The three coolest waste packages are all DHLW waste packages. The three hottest waste packages are all PWR waste packages. The old PWR waste package and BWR waste packages fall in the middle of the temperature range. The reduction in relative humidity on waste packages correlates directly with temperature on the waste package. Therefore the PWR waste packages always experience the greatest relative humidity reduction, while the DHLW waste packages experience the least relative humidity reduction. At late times there is a greater range of relative humidity reduction resulting from waste package-to-waste package variability than arising from the distance from the potential repository edges (compare Figures 5.4.1-7b and 5.4.1-2d).

The HTOM thermal-hydrologic results were abstracted and provided to TSPA (Francis and Itamura 2001 [DIRS 155321]) for use in SSPA Volume 2 (McNeish 2001 [DIRS 155023]).

5.4.2 Lower Temperature Operating Mode Base Case Results

This section describes the multiscale thermal-hydrologic (MSTH) model base-case calculations (Buscheck 2001 [DIRS 155243]) for the LTOM, which includes the mean, upper, and lower infiltration-flux scenarios. Figure 5.4.2-1 gives the plan view of the MSTH model representation of the potential LTOM repository; also shown are the geographic locations for which TH conditions are given in Figures 5.4.2-2 and 5.4.2-3. The potential LTOM repository area is 20 percent larger than the potential HTOM repository (Figure 5.4.1-1). These locations were chosen to illustrate the manner in which TH behavior is influenced by proximity to the edges of the potential repository. Four of these locations are close to the center of the potential repository; two are located in the extreme northeast and southwest corners of the potential repository area, and two are at the extreme eastern and western edges of the area, approximately midway between the northern and southern boundaries. The temperature and relative-humidity histories fall into three distinct clusters (one for the potential repository-center locations, one for the potential repository corners, and one for the potential repository-edge locations), and the reduction in relative humidity can be classified into two sequential periods (Figure 5.4.2-2).

An early-to-intermediate period lasts for about 20,000 years, during which time heat-transfer in the drift controls the magnitude of the reduction in relative humidity on waste packages. Because the temperatures for the LTOM are always below the boiling point of water, there is no rock dryout period, and no reduction in relative humidity in the host rock (Figure 5.4.2-2c); therefore, all reductions in relative humidity on waste packages arise as a result of the temperature differences, $\Delta T_{wp\text{-}dw}$, between waste packages and the drift wall. The early-to-intermediate period for the LTOM case has the same trends as observed for the intermediate period for the HTOM case (Section 5.4.1). During this period, the reduction in relative humidity on waste packages decreases with distance from the potential repository edges.

A late period, beginning around 20,000 years, occurs during which the reduction in relative humidity on waste packages becomes decreasingly sensitive to proximity to the potential repository edges. For a given waste-package type, the reduction in relative humidity becomes increasingly similar across the potential repository area.

Figure 5.4.2-4 shows the influence of the edge-cooling effect, with locations close to the potential repository edges cooling more quickly than those at the center. Figure 5.4.2-5 also shows the trend of the reduction in relative humidity on waste packages increasing with proximity to the potential repository edges.

Figures 5.4.2-3a and 5.4.2-3b show the relationship between liquid saturation in the invert and evaporation rate. At the end of the ventilation period, the invert is assumed to be dry in the model. Rewetting of the invert begins immediately after the end of the ventilation period, which occurs at 300 yr. Therefore, evaporation rates in the invert are always nonzero. Rewetting of the invert occurs more quickly at potential repository-edge locations than at potential repository-center locations because the edge-cooling effect reduces the amount of heating available to evaporate the incoming water. At 300 yr, an initial spike is seen in the evaporation rate as the liquid-phase flux into the invert immediately increases following the end of the ventilation period. The two geographic locations that experience a larger eventual increase in liquid saturation in the invert correspond to the two locations wherein the local host rock is either the middle or lower non-lithophysal Topopah Spring welded tuff unit (Tptpmn or Tptpln). Wherever the local host-rock unit is comprised of the lower lithophysal unit (Tptpll), the maximum liquid saturation in the invert is nearly the same (and lower than in locations where the local host-rock unit is Tptpmn or Tptpln). Apparently, there is a difference in re-wetting behavior in the invert that depends on the local host-rock unit. The second spike in the invert evaporation rate occurs shortly after 600 yr when a substantial increase in infiltration flux occurs. The increase in infiltration rate is accompanied by an increase in liquid-phase flux into the invert, which makes more water available for evaporation in the invert.

Figure 5.4.2-6 gives the complementary cumulative distribution functions for temperature and relative humidity on the waste package for the mean, lower, and upper infiltration-flux scenarios. For the mean-infiltration-flux scenario, the peak waste package temperatures range from 64.9° to 91.2°C. For the low-infiltration-flux scenario, the temperatures are higher than in the mean-infiltration-flux scenario, ranging from 66.1° to 93.3°C. The upper infiltration-flux scenario results in lower peak waste package temperature that ranges from 64.4° to 90.6°C.

Figure 5.4.2-6b, which gives the complementary cumulative distribution function of the time required for waste packages to attain a relative humidity of 80 percent show a distinct change in the slope of the curves at a complementary cumulative distribution function value of 0.7; this sharp break in the slope of the complementary cumulative distribution function curves indicates that there are two distinctively different groups of waste packages with respect to the duration of relatively dry relative humidity on the waste-package surfaces. In the MSTH model (Buscheck 2001 [DIRS 155243]), 30 percent of the waste packages are DHLW waste packages and 70 percent are CSNF waste packages. A detailed inspection of the underlying data that is plotted in Figure 5.4.2-6b shows that the break in slope at a complementary cumulative distribution function value of 0.7 correspond with the fact that 30 percent of the waste-package inventory that attains an relative humidity of 80 percent first (i.e., having a complementary cumulative distribution function value between 0.7 and 1.0) is entirely comprised of DHLW waste packages. Those waste packages that have a complementary cumulative distribution function value between 0.0 and 0.7 are entirely comprised of CSNF waste packages. Thus, all of the DHLW waste packages have a relatively short duration of reduced relative humidity, requiring less than 1,418 years to attain a relative humidity of 80 percent. All CSNF (PWR and BWR) waste packages require at least 2,091 years to attain a relative humidity of 80 percent; the driest PWR requires 8,982 years to attain a relative humidity of 80 percent.

The time required for the waste package to attain a relative humidity of 80 percent is similar for the mean and lower-infiltration flux scenarios (Figure 5.4.2-6b). Because rock dryout does not occur, the reduction in relative humidity depends entirely on multi-scale heat flow occurring in the rock at the mountain scale and within the drift at the waste package scale. The upper-infiltration-flux scenario results in a more persistent relative humidity reduction on waste packages because the cooler temperatures associated with this scenario result in less efficient thermal radiative heat transfer in the drifts, which causes a larger $\Delta T_{wp\text{-}dw}$ between the waste package and drift wall. Also, the reduction in relative humidity arising from $\Delta T_{wp\text{-}dw}$ is more effective at lower temperatures, as was observed for potential repository-edge locations. The waste package temperature at the time when the relative humidity reaches 80 percent on the waste package is highest for the lower-infiltration-flux scenario and lowest for the upper infiltration-flux scenario (Figure 5.4.2-6c).

The LTOM results in a more persistent relative humidity reduction on waste packages than does the HTOM (compare Figure 5.4.2-6b with Figure 5.4.1-6c). Moreover, the LTOM results in lower waste package temperatures at 80 percent relative humidity than does the HTOM (compare Figure 5.4.2-6c with Figure 5.4.1-6d). In general, the LTOM case results in lower waste package temperatures at any given value of relative humidity on the waste package than does the HTOM case.

Figure 5.4.2-7 shows the waste package-to-waste package variability in temperature and relative humidity at a location in the potential repository that is relatively close to the geographic center. Peak waste package temperatures range from 78.1° to 91.2°C. The three coolest waste packages are all DHLW waste packages. The three hottest waste packages are all PWR waste packages. The old PWR waste package and BWR waste packages fall in the middle of the temperature range. The reduction in relative humidity on waste packages correlates directly with temperature on the waste package. Therefore the PWR waste packages always experience the greatest reduction in relative humidity, while the DHLW waste packages experience the smallest reduction in relative humidity. At late times, there is a greater range of relative humidity reduction resulting from waste package-to-waste package variability than arising from the distance from the potential repository edges (compare Figure 5.4.2-7b with Figure 5.4.2-2d).

Figure 5.4.2-8 compares the TH conditions on typical PWR waste package surfaces for the HTOM and LTOM cases. All geographic locations (edge, corner, and center) are included within the shaded regions for the two operating modes. The bands of the TH conditions represent the progression in time, ending at ambient conditions of about 25°C and 100 percent relative humidity. The LTOM results in lower relative humidity for any given temperature, or lower temperature for any given relative humidity for all locations except for the corner of the potential repository where the HTOM results in lower relative humidity or temperature than the central LTOM locations.

The LTOM thermal-hydrologic results were abstracted and provided to TSPA (Francis and Itamura 2001 [DIRS 155321]) for use in Volume 2 (McNeish 2001 [DIRS 155023]).

5.4.3 Process Model Results

Section 5.3.1 evaluated the multiscale model for in-drift hydrologic conditions, while Section 5.3.2 evaluated ventilation and convection modeling of in-drift thermal-hydrologic conditions. Quantification of uncertainties related to in-drift hydrologic conditions and to ventilation and convection evaluations are presented in Sections 5.3.1.4 and 5.3.2.4, respectively, based on the process models used to investigate the sensitivity of in-drift TH performance to a number of uncertainties and parameters. Each of those sections includes a short summary of the results of the sensitivity calculations.

In this section, the results of the sensitivity studies are compared to determine which parameters and uncertainties are most important for in-drift TH performance. Table 5.4.3-1 shows the results of the sensitivity studies. The table indicates which uncertainty is dealt with in each subsection and lists the parameter or uncertainty range considered in the sensitivity studies. When a sensitivity study evaluated the effects of considering or not considering the parameter in the analyses rather than considering a range of values, this is indicated as include or exclude. The table indicates the values used in the base case analyses (or whether the parameter was included or excluded), the performance measures considered, and what the results of the sensitivity studies indicated were the effects of the range of parameter values or uncertainty on the performance measure.

Analyses were conducted using the submodels of the multiscale thermal-hydrologic model, to consider the sensitivity to operational parameters, and the sensitivity to the uncertainty and variability of properties of the natural and engineered systems. These analyses considered both the HTOM and LTOM cases. The focus was on the effects of heat-driven coupled-processes on in-drift thermal-hydrologic conditions. The TH conditions considered include temperature and relative humidity at the waste packages and drip shield, and saturation at the drift wall and in the invert.

Peak temperatures at the drip shield and waste package were most sensitive to ventilation parameters and to thermal conductivity values used in the models. The uncertainty in host rock thermal conductivity had the most significant effect. The drift wall and drip shield peak temperatures had a range of 85 and 20°C (for the HTOM and LTOM) resulting from a thermal conductivity range of 1.13-2.01 W/m•K (saturated) and 0.54-1.54 W/m•K (dry). The key factor determining the spatial variability of thermal conductivity is the variability of lithophysal porosity. The range of drift wall and drip shield temperatures was about 100 and 25°C (for the HTOM and LTOM) when a range of 0 to 25 percent of lithophysal porosity was used. The increase in temperature was due to the additional effect of porosity on heat capacity, in addition to the effect on thermal conductivity.

The second most significant factors were those related to ventilation. There was a range of about 60°C (for both the HTOM and LTOM) in pre-closure peak drip shield temperatures resulting from using constant versus time-dependent ventilation efficiency. A 14 and 7°C postclosure drip shield temperature range (for the HTOM and LTOM) resulted from a 20 percent variation in ventilation efficiency (heat removal). For the LTOM, it was concluded that a 44-year variability in ventilation duration from one part of the potential repository to another would have only a minor effect on postclosure temperatures.

The significant uncertainties resulting from using 2D analyses were also quantified. The detailed 3D analyses of in-drift TH effects calculated 26 and 8°C ranges (for the HTOM and LTOM) in postclosure peak temperatures from the hottest to the coolest waste packages.

The ventilation efficiency was calculated using two independent models, and compared to the quarter-scale tests. The models, which used a wide range of convective heat transfer coefficients, bracketed the measured results. The influence of water entering the drift and evaporating into the dry ventilation air was not significant on overall ventilation efficiency, and had only a minor effect on ventilation air humidity.

A number of other parameters were investigated, including the effect of lithophysal porosity on gas storage, seepage effects on in-drift humidity, imbibition hysteresis, buoyant gas-phase convection in the rock, THC and THM processes, host rock permeability, invert conductivity, and treatment of thermal radiation and natural convection in the drift. These parameters had only small effects on the magnitude of in-drift temperatures. However, the invert conductivity and the sophistication of natural convection models were found to influence which part of the EBS are cooler than others, with potential influence on formation of condensate which could be the source for corrosion or transport.

Finally, multiple approaches to achieving LTOM temperatures were evaluated. Derating PWR waste packages was the most effective method of reducing peak temperatures, followed by drift spacing (for line-loaded drifts), and finally, waste package spacing. However, the range of temperatures among these methods was small (within 3°C); therefore, other factors such as worker safety or cost should be considered when selecting a license application design for lower-temperature operation.

Summary–In general the model results considered in Section 5 have provided: 1) additional understanding of recognized uncertainties associated with thermal-hydrologic modeling as implemented in the MSTH model and ventilation models; 2) increased confidence in predicted temperature, relative humidity, and other measures of the in-drift environment over a range of thermal conditions bounded by the assumed HTOM and LTOM, and 3) increased confidence in the results of the TSPA-SR. Those results that use the more detailed process models are an additional line of evidence from the TSPA (abstracted) model results.

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Table 5.1-1. Design Parameters Used in Sensitivity Studies to Address Three Operational Modes

Design feature	Higher-Temperature Operation Mode (above boiling repository)	96°C Drift Wall (Not Analyzed)	Lower-Temperature Operating Mode (85°C Waste Package)
Drift spacing	81 m	81 m	81 m
Areal Mass Loading	54.5 MTU/acre	54.5 MTU/acre	45.7 MTU/acre
Repository footprint	4.65 km^2	4.65 km^2	5.58 km^2
Lineal Power density	1.35 kW/m	1.35 kW/m	1.13 kW/m
Length of Ventilation	50 yrs forced	300 yrs forced	300 yrs forced
Heat removal by Ventilation	70 %	80%	80%
Waste Package configuration/spacingation	Line load, 10 cm	Line load, 10 cm	Line/point load, gaps from 10 cm to 2.8 m

Source: BSC 2001 [DIRS 154864].

Table 5.2-1. Near Field Environment and Engineered Barrier System Thermal-Hydrologic Variables Calculated with the Multiscale Thermal-Hydrologic Model at 610 Repository Locations for No-Backfill Realizations

Thermal-Hydrologic Variable	Drift-Scale Location
Near Field Environment Parameters	
Temperature	Near Field Environment rock (5 m above drift and along the entire repository horizon)
	Maximum lateral extent of boiling
	Upper drift wall (crown of the drift)
	Lower drift wall (below invert)
	Drift wall (perimeter average)
Relative Humidity	Drift-wall (perimeter average)
Liquid-phase matrix saturation	Drift wall (perimeter average)
Liquid-phase flux	Near Field Environment host rock (5 m and 3 m above crown of drift)
	Drift-wall (upper surface perimeter average in matrix & fractures)
Gas-phase (water vapor) flux	Drift wall (perimeter average)
Gas-phase (air) flux	Drift wall (perimeter average)
Evaporation rate	Near Field Environment rock (5 m above drift)
Engineered Barrier System Parameters	
Temperature	Drift wall (perimeter average)
	Drip shield (perimeter average and upper surface)
	Waste Package (surface average)
	Invert (average)
Relative humidity	Drift-wall (perimeter average)
	Backfill (crown)
	Drip shield (perimeter average)
	Waste package
	Invert (average)

Table 5.2-1. Near Field Environment and Engineered Barrier System Thermal-Hydrologic Variables Calculated with the Multiscale Thermal-Hydrologic Model at 610 Repository Locations for No-Backfill Realizations (Continued)

Thermal-Hydrologic Variable	Drift-Scale Location
Engineered Barrier System Parameters	
Liquid-phase matrix saturation	Drift wall (perimeter average)
	Invert (average)
Liquid-phase flux	Drip shield (crown, upper surface average, and lower side at the base)
	Invert (average)
Gas-phase air-mass fraction	Drip shield (perimeter average)
Gas-phase pressure	Drip shield (perimeter average)
Capillary Pressure	Invert (average)
	Drift wall (crown, in matrix and in fractures)
Gas-phase (water vapor) flux	Drift wall (perimeter average)
Gas-phase (air) flux	Drift wall (perimeter average)
Evaporation Rate	Drip shield (perimeter total and crown) (calculated during the abstraction)
	Invert (total)

Source: Modified from CRWMS 2000 [DIRS 153363], Table 3-6.

Table 5.3.1.2-1. Key Thermal-Hydrologic Uncertainties

Model (Conceptual) Uncertainty (Section 5.3.1.2.1)	Process Uncertainty (Section 5.3.1.2.2)	Input Data Uncertainty (Section 5.3.1.2.3)
Use of effective thermal conductivity and thermal radiation approaches		
Porous media approximation of comprehensive fluid dynamics processes	Hysteresis of imbibition	Invert properties
Use of single continuum versus DKM approach for invert materials	THM and THC changes to hydrologic properties	Host rock bulk permeability
Neglecting dryout during ventilation		Host rock thermal conductivity
Coupling of submodels		Host rock heat capacity
Localized effects of seepage		Heat output of waste packages
Neglecting fracture heterogeneity impacts on seepage		Impacts of lithophysal porosity on thermal conductivity
Neglecting effects of mountain-scale gas-phase convection		Wet and dry thermal conductivity
Effects of lithophysal porosity on vapor storage		Duration of ventilation

Source: Developed for this document.

NOTE: DKM = dual permeability mode
THM = thermal-hydrologic-mechanical
THC = thermal-hydrologic-chemical.

Table 5.3.1.4.2-1. Statistical Parameters Used in the Three-Dimensional, Heterogeneous Line-Averaged-Heat-Source, Drift-Scale Thermal-Hydrologic Model Realizations

Stochastic Realization	**Standard Deviation of *k* (log_{10})**	**Correlation Length (m)**			**van Genuchten Alpha Value Correlated to *k***
		Lateral (x)	**Axial (y)**	**Vertical (z)**	
A-56	1.5	0.5	0.5	4.0	yes
A-34	1.5	0.5	0.5	4.0	yes
B-56	1.5	0.5	0.5	4.0	no
B-34	1.5	0.5	0.5	4.0	no
C-56	1.0	1.0	1.0	1.0	yes
C-34	1.0	1.0	1.0	1.0	yes
D-56	2.3	1.0	1.0	2.0	yes
D-34	2.3	1.0	1.0	2.0	yes

Source: BSC 2001 [DIRS 155007], Table 6-8.

Table 5.3.1.4.2-2. Summary of Seepage Conditions When TH Conditions Have Returned to Near-Ambient (Glacial Climate)

Stochastic Realization	**Seepage Percentage Entering Drift (%)**	**Seepage Percentage Contacting Drip Shield (%)**
A-56	37.5	30.4
A-34	54.8	13.6
B-56	27.9	0.1
B-34	21.3	4.4
C-56	0.0	0.0
C-34	0.0	0.0
D-56	42.9	11.0
D-34	85.5	26.4

Source: BSC 2001 [DIRS 155007], Table 6-10.

NOTE: Seepage percentage is the fraction of the incident average percolation flux.

Table 5.3.1.4.6-1. Input Parameters and Data Tracking Numbers for Distinct Element Analysis

Description	Value	Units	Data Tracking Number (DTN)
Matrix properties			
Dry bulk density	2,270	kg/m^3	MO0010RDDAAMRR.002 [DIRS 154048]
Intact rock elasticity modulus	33.03	GPa	MO9911SEPGRP34.000 [DIRS 148524]
Rock mass elasticity modulus	24.71	GPa	MO9911SEPGRP34.000 [DIRS 148524]
Poisson's ratio	0.21	none	MO9911SEPGRP34.000 [DIRS 148524]
Joint properties			
Joint friction	41	degrees	MO0003SEPDRDDA.000 [DIRS 147607]
Joint cohesion	0.09	MPa	MO9911SEPGRP34.000 [DIRS 148524]
Joint dilation angle	29	degrees	MO9911SEPGRP34.000 [DIRS 148524]
Initial joint aperture	0.098	mm	LB990501233129.001 [DIRS 106787]
Thermal properties			
Thermal expansion coefficient	9.73E-6	degrees C^{-1}	MO0004RIB00035.001 [DIRS 153848]
Stress and stress gradient			
In situ stress (at 380m depth)	7.6	MPa	MO0007RIB00077.000 [DIRS 154087]
Vertical stress gradient	0.023	MPa/m	MO0007RIB00077.000 [DIRS 154087]
Input temperature			
Input temperatures	various	degrees C	LL000114004242.090 [DIRS 142884]

Source: Blair 2001 [DIRS 155005], Table 2.

Table 5.3.1.4.6-2 Comparison of Range of Bulk (Fracture) Permeability Values for Geologic Units Considered in Multiscale Thermal-Hydrologic Model Sensitivity Studies to Potential Range from THM Effects

Geologic Unit	Mean Value of Permeability (k), m^2 (As Reported in Table 5.3.1.4.7-1)	Variability of Permeability in Thermal-Hydrologic Sensitivity Studies: Permeability Range Considered in Effects of Bulk Permeability, m^2 (Section 5.3.1.4.7)*	Variability of Permeability in Thermal-Hydrologic Sensitivity Studies: Range of Permeability Considered in Seepage Analyses (Section 5.3.1.4.2)	Potential Changes From Mean *k* Due to THM
tsw32	2.51 E-12	1.58 E-13 3.98E-11		2.5 E-17 1.5 E-11
33	8.79 E-13	5.55 E-14 1.39 E-11		8.8 E-18 5.3 E-12
34	3.68E-13	2.32 E-14 5.83 E-12		3.7 E-18 2.2 E-12
35**	2.38 E-12	1.50 E-12 3.77 E-13	2.9 E-14 2.8 E-11	2.4E-17 1.4 E-11
36/37	1.38 E-12	8.71 E-13 2.19E-12		1.4 E-17 8.3 E-12

Source: The last column was produced by multiplying column two by six and dividing by 100,000, applying the results of Blair 2001 [DIRS 155005], Section 6.3.3.

NOTE: * = ± 2 standard deviations from mean
** = lower lithophysal subunit.

Table 5.3.1.4.6-3. Summary of Thermal-Hydrologic-Mechanical Simulations of the Large Block Test

Simulation #	Number of Fractures	CTE (per °C)	Description
1	0	5.27 E-06	Continuum model
2	6	9.73 E-06	High CTE with 6 major fractures
3	6	5.27 E-06	Low CTE with 6 major fractures
4	7	5.27 E-06	Same as 3 with one additional fracture
5	28	5.27 E-06	Additional fractures included in fracture analysis

Source: Produced using files from Blair 2001 [DIRS 155309].

NOTE: CTE = coefficient of thermal expansion.

Table 5.3.1.4.7-1. Bulk (Fracture) Permeability Values for Geologic Units used in the Multiscale Thermal-Hydrologic Model Analyses, Along with the Assumed Value of Sigma used in the Sensitivity Study of k_b

Unit	Permeability (k), m^2	log(k)	sigma (log k_b)	two sigma (log k_b)
tsw32	2.51e-12	-11.600	0.60	1.2
33	8.79e-13	-12.056	0.60	1.2
34	3.68e-13	-12.434	0.60	1.2
35	2.38e-12	-11.623	0.60	1.2
36/37	1.38e-12	-11.860	0.60	1.2

Source: Produced using files from Buscheck 2001 [DIRS 155243].

NOTE: No sigmas for tsw31 or 38/39. The high and low k_b cases assumed one sigma and that the very high and very low k_b cases assume two sigma deviation from the mean k_b value.

Table 5.3.1.4.8-1. Lithophysal Unit Thermal Conductivity Values Used in the MSTH Model Sensitivity Analyses

K_{th} Case	Lithophysal Porosity		Saturated Thermal Conductivity (W/m•K)		Dry Thermal Conductivity (W/m•K)	
	Lower Lithophysal Unit, Tptpll	Upper Lithophysal Unit, Tptpul	Lower Lithophysal Unit, Tptpll	Upper Lithophysal Unit, Tptpul	Lower Lithophysal Unit, Tptpll	Upper Lithophysal Unit, Tptpul
High K_{th}	0%	5%	2.02	2.13	1.54	1.43
Mean K_{th}	12.5%	21.6%	1.87	1.55	1.27	0.84
Low K_{th}	25%	38%	1.13	0.74	0.64	0.31

Source: Adapted from BSC 2001 [DIRS 155008].

Table 5.3.1.4.8-2. Comparison of Relative Humidity Conditions on Drift Wall as Function of K_{th} for the Higher-Thermal Operating Mode Case

K_{th}	RH at 50-60 years post-emplacement	RH at 400 years post-emplacement	RH at 1000 years post-emplacement	Time to reach 60% Relative Humidity	Time to reach 95% Relative Humidity
High K_{th}	28%	70%	100%	280 years	700 years
Mean K_{th}	20%	60%	95%	400 years	1000 years
Low K_{th}	3-5%	23%	60%	1000 years	2000 years

Source: Produced using files from Buscheck 2001 [DIRS 155243].

Table 5.3.1.4.9-1. Lithophysal Porosity Values used in MSTH Model Sensitivity Analyses

K_{th} Case	Lithophysal Porosity	
	Lower Lithophysal Unit, Tptpll	Upper Lithophysal Unit, Tptpul
High K_{th}	0%	5%
Mean K_{th}	12.5%	21.6%
Low K_{th}	25%	38%

Source: Produced using files from BSC 2001 [DIRS 155008], Table 24.

Table 5.3.1.4.10-1. Thermal Conductivity in the Upper Half of the Invert for the Sensitivity Calculation

Case	Nominal Thermal Conductivity (W/m•K)	First Continuum Thermal Conductivity (W/m•K)	Second Continuum Thermal Conductivity (W/m•K)
Base (no steel credit)	0.15	0.075	0.075
Intermediate	0.835	0.76	0.075
As-built	1.52	0.76	0.76
Additional steel	3.04	1.52	1.52

Source: Produced using files from Reed 2001 [DIRS 155076].

Table 5.3.1.4.10-2. Calculated Peak Temperatures for Each Invert Conductivity

EBS Locations	Temperature (°C) Resulting From The Invert Conductivity			
	Base	Intermediate	As-Built	Additional Steel
Drift wall crown	147	146	145	145
Drift wall rib	150	148	148	147
Invert lower-center	143	150	152	152
Drip shield top	161	159	159	158
Drip shield base	163	160	160	159

Source: Produced using files from Reed 2001 [DIRS 155076].

Table 5.3.1.4.11-1. Waste Package Peak Temperatures for the Three Lower-Temperature Operating Mode Sensitivity Cases

Case	Design Parameters	Operational Parameters	Fraction of Waste Packages with Peak Temperature >85°C (Full MSTH Results)	Peak Waste Package Temperature (Full MSTH Results)	Peak Waste Package Temperature (L5C3 MSTH Results)
LTOM-PA Base Case	5.5 m drift diameter 81 m drift spacing 21 PWR WPs	15 m^3/s ventilation for 300 yr, 1.1 m average WP spacing	38%	91.2°C	90.0°C
Wider Drift Spacing	5.5 m drift diameter 97 m drift spacing 21 PWR WPs	15 m^3/s ventilation for 300 yr, 0.1 m WP spacing	Not calculated	Not calculated	88.8°C
De-rated WP Capacity	5.5 m drift diameter 81 m drift spacing 16 PWR WPs	15 m^3/s ventilation for 300 yr, 0.1 m WP spacing	26%	87.9°C	87.3°C

Source: Produced using files from Buscheck 2001 [DIRS 155243].

NOTES: The three sensitivity cases use the full MSTH model and a simplified implementation of the MSTH model at a single location in the repository footprint.

PWR = pressurized water reactor; MSTH = multiscale thermal-hydrologic; WP = waste package.

Table 5.3.2.4.1-1. Preclosure Temperatures and Ventilation Efficiencies Calculated with Two Models

Parameter	10 m^3/s		15 m^3/s	
	ANSYS	MULTIFLUX	ANSYS	MULTIFLUX
Peak Drift Wall Temperature	94°C	93°C	76°C	71°C
Peak Air Temperature	79°C	85°C	64°C	67°C
Average Efficiency, 50-yr duration	68%	91%	74%	94%
Average Efficiency, 100-yr duration	73%	93%	78%	95%
Average Efficiency, 200-yr duration	77%	96%	82%	97%

Source: Produced from information in CRWMS M&O 2000 [DIRS 120903] and BSC 2001 [DIRS 155025].

Table 5.3.2.4.1-2. Fraction of Total Heat Removal via Ventilation Due to Latent Heat of Water Vaporized from the Near-Field Rock

Period From Start of Ventilation (year)	Average Latent Heat Removal During the Period (% of Total Heat Removal by Ventilation)	
	10 m^3/s	15 m^3/s
0.5	1.93%	0.99%
5	2.82%	1.38%
25	2.21%	1.35%
50	1.98%	1.30%
100	1.95%	1.31%
200	2.08%	1.43%
300	2.24%	1.55%

Source: Produced from information in BSC 2001 [DIRS 155025].

Table 5.3.2.4.2-1. Summary of HTOM Thermal-Hydrologic Parameter Sensitivity to Ventilation Efficiency

Case	Time-Averaged Ventilation Efficiency	Drip Shield Top Peak Preclosure Temperature (°C)	Drip Shield Top Peak Postclosure Temperature (°C)	Drift Wall Crown Peak Temperature (°C)	Time for Drip Shield Top RH > 50 % (year)	Time for Drift Wall Crown RH > 50 % (year)
-10%	60%	117	166	153	460	320
Base case	70%	94	158	146	400	280
Averaged f(t)	73%	87	156	144	380	260
f(t)	73%	146	155	143	380	260
+10%	80%	70	152	139	340	240

Source: Produced using files from Leem 2001 [DIRS 154996].

Table 5.3.2.4.2-2. Summary of Lower-Temperature Operating Mode Thermal-Hydrologic Parameter Sensitivity to Ventilation Efficiency

Case	Time-Averaged Ventilation Efficiency	Drip Shield Top Peak Preclosure Temperature (°C)	Drip Shield Top Peak Postclosure Temperature (°C)	Drift Wall Crown Peak Temperature (°C)
-10%	70%	82	84	75
Base case	80%	63	80	72
Averaged f(t)	83%	57	79	71
f(t)	83%	120	79	70
+10%	90%	43	77	68

Source: Produced using files from Leem 2001 [DIRS 154996].

Table 5.3.2.4.3-1. Summary of Lower-Temperature Operating Mode Thermal-Hydrologic Parameter Sensitivity to Ventilation Duration

Case	Ventilation Duration	Drip Shield Top Preclosure Temperature (°C)	Drip Shield Top Peak Postclosure Temperature (°C)	Drift Wall Crown Peak Temperature (°C)
Shorter Ventilation Duration	278 years	63	82	73
Base case	300 years	63	80	72
Longer Ventilation Duration	322 years	63	79	71

Source: Produced using files from Leem 2001 [DIRS 154996].

Table 5.3.2.4.5-1. Bulk Permeabilities for In-Drift Air

Case Study	Bulk Permeability (m^2)
Low value	0
Fracture-permeability-limited	4.76×10^{-12}
Base case	10^{-8}
High value	2×10^{-5}

Source: Produced using files from Francis 2001 [DIRS 155075].

Table 5.3.2.4.6-1. In-Drift Temperatures for the Higher-Temperature Operating Mode

Location	Temperature, °C						
	10 yr*	51 yr	65 yr**	200 yr	1000 yr	2000 yr	100,000 yr***
Design Basis PWR WP							
Waste Pkg Upper Half	119.9	166.2	184.5	154.8	134.2	114.2	26.9
Waste Pkg Lower Half	123.3	171.3	188.5	156.7	134.9	114.6	27.0
Drip Shield Top-Center	107.8	150.9	173.3	149.0	131.9	112.8	26.8
Drip Shield Top-Corner	105.2	147.5	170.7	147.7	131.5	112.6	26.8
Drip Shield Bottom-Corner	106.7	149.8	172.5	148.5	131.8	112.7	26.8
Drift Wall Crown	98.4	139.1	164.9	144.8	130.4	111.9	26.7
Drift Wall 1:30	98.8	139.8	165.4	145.0	130.4	111.9	26.7
Drift Wall Rib	99.2	140.3	165.8	145.2	130.5	112.0	26.7
Drift Wall 4:30	99.3	140.4	165.9	145.3	130.5	112.0	26.8
Invert Top-Center	119.6	166.7	185.1	154.9	134.2	114.2	26.9
Invert Top-Right	101.5	143.2	167.9	146.2	130.9	112.2	26.8
Average WP (BWR)							
Waste Pkg Upper Half	112.1	156.6	177.3	152.0	133.2	113.7	26.9
Waste Pkg Lower Half	114.6	160.3	180.2	153.3	133.7	114.0	26.9
Drip Shield Top-Center	103.3	145.9	169.7	148.3	131.8	112.7	26.8
Drip Shield Top-Corner	101.6	143.6	168.0	147.5	131.5	112.5	26.8
Drip Shield Bottom-Corner	102.5	145.1	169.1	148.0	131.6	112.6	26.8
Drift Wall Crown	96.1	137.0	163.5	145.3	130.6	112.0	26.7
Drift Wall 1:30	96.5	137.6	163.9	145.5	130.7	112.0	26.7
Drift Wall Rib	96.7	137.8	164.0	145.6	130.7	112.0	26.7
Drift Wall 4:30	96.4	137.5	163.8	145.4	130.7	112.0	26.8
Invert Top-Center	112.1	157.4	178.1	152.2	133.3	113.7	26.9
Invert Top-Right	98.4	139.9	165.5	146.3	131.0	112.2	26.8
Cool WP (DHLW)							
Waste Pkg Upper Half	92.8	130.8	158.5	142.3	129.5	111.4	26.7
Waste Pkg Lower Half	93.2	131.3	158.8	142.5	129.6	111.5	26.7
Drip Shield Top-Center	91.7	129.6	157.7	142.0	129.4	111.4	26.7
Drip Shield Top-Corner	91.4	129.2	157.4	141.9	129.4	111.3	26.7
Drip Shield Bottom-Corner	91.1	128.8	157.2	141.8	129.3	111.3	26.7
Drift Wall Crown	89.4	126.7	155.7	141.1	129.1	111.1	26.6
Drift Wall 1:30	89.5	126.9	155.9	141.2	129.1	111.2	26.6

Table 5.3.2.4.6-1. In-Drift Temperatures for the Higher-Temperature Operating Mode (Continued)

Location	Temperature, °C						
	10 yr*	**51 yr**	**65 yr****	**200 yr**	**1000 yr**	**2000 yr**	**100,000 yr*****
Cool WP (DHLW)							
Drift Wall Rib	89.2	126.5	155.6	141.1	129.1	111.1	26.7
Drift Wall 4:30	88.5	125.5	154.8	140.7	129.0	111.1	26.7
Invert Top-Center	93.0	131.1	158.8	142.5	129.6	111.5	26.7
Invert Top-Right	89.7	127.1	156.0	141.3	129.2	111.2	26.7

Source: Produced using files from Buscheck 2001 [DIRS 155243].

NOTE: * = Time of Preclosure Peak T
** = Time of Postclosure Peak T
*** = Near-Ambient T.

Table 5.3.2.4.6-2. In-Drift Temperatures for the Lower-Temperature Operating Mode (Page 1 of 2)

Location	Temperature, °C						
	10 yr*	**301 yr**	**500 yr**	**780 yr****	**1000**	**4000**	**100,000*****
Design Basis PWR WP							
Waste Pkg Upper Half	84.6	76.2	97.4	98.4	97.0	73.8	26.5
Waste Pkg Lower Half	86.8	77.9	98.6	99.3	97.7	74.1	26.5
Drip Shield Top-Center	73.3	67.2	91.8	94.4	93.8	72.4	26.4
Drip Shield Top-Corner	70.6	65.0	90.5	93.5	93.0	72.0	26.3
Drip Shield Bottom-Corner	71.5	65.8	91.0	93.9	93.3	72.2	26.4
Drift Wall Crown	63.2	59.3	87.1	91.2	91.1	71.2	26.2
Drift Wall 1:30	63.5	59.5	87.3	91.3	91.2	71.2	26.3
Drift Wall Rib	64.1	60.0	87.5	91.5	91.4	71.3	26.3
Drift Wall 4:30	64.4	60.3	87.7	91.6	91.4	71.3	26.3
Invert Top-Center	83.1	74.9	96.7	98.0	96.6	73.6	26.5
Invert Top-Right	66.9	62.2	88.8	92.4	92.1	71.6	26.4
Average WP (BWR)							
Waste Pkg Upper Half	75.6	67.9	92.0	94.7	94.1	72.7	26.4
Waste Pkg Lower Half	77.3	69.1	92.8	95.3	94.6	73.0	26.4
Drip Shield Top-Center	68.2	62.6	88.8	92.4	92.2	71.8	26.3
Drip Shield Top-Corner	66.7	61.5	88.1	91.9	91.8	71.6	26.3
Drip Shield Bottom-Corner	67.4	62.0	88.4	92.2	92.0	71.7	26.3
Drift Wall Crown	62.6	58.5	86.4	90.7	90.8	71.2	26.2
Drift Wall 1:30	62.8	58.7	86.5	90.8	90.8	71.2	26.2
Drift Wall Rib	63.0	58.8	86.5	90.8	90.9	71.2	26.3
Drift Wall 4:30	62.9	58.7	86.5	90.8	90.9	71.2	26.3
Invert Top-Center	74.9	67.3	91.8	94.6	93.9	72.7	26.4
Invert Top-Right	64.3	59.8	87.1	91.2	91.2	71.4	26.3
Hot Gap							
Drip Shield Top-Center	67.8	61.9	88.0	91.8	91.7	71.6	26.3
Drip Shield Top-Corner	66.8	61.2	87.6	91.5	91.5	71.5	26.3
Drip Shield Bottom-Corner	67.2	61.5	87.8	91.7	91.6	71.5	26.3
Drift Wall Crown	64.0	59.0	86.3	90.6	90.7	71.2	26.2
Drift Wall 1:30	64.1	59.1	86.4	90.7	90.8	71.2	26.2
Drift Wall Rib	64.1	59.1	86.4	90.7	90.8	71.2	26.3
Drift Wall 4:30	63.8	58.9	86.2	90.6	90.7	71.2	26.3
Invert Top-Center	70.9	64.3	89.5	92.9	92.6	72.0	26.4
Invert Top-Right	64.9	59.8	86.8	91.0	91.0	71.3	26.3

Source: Produced using files from Buscheck 2001 [DIRS 155243].

NOTE: * = Time of Preclosure Peak T
** = Time of Postclosure Peak T
*** = Near-Ambient T.

Table 5.3.2.4.6-2. In-Drift Temperatures for the Lower-Temperature Operating Mode (Page 2 of 2)

	Temperature, °C						
Location	**10 yr***	**301 yr**	**500 yr**	**780 yr****	**1000 yr**	**4000 y**	**100,000*****
Cool Gap							
Drip Shield Top-Center	66.1	59.2	86.1	90.5	90.6	71.2	26.3
Drip Shield Top-Corner	65.1	58.6	85.7	90.2	90.4	71.1	26.3
Drip Shield Bottom-Corner	65.3	58.6	85.7	90.2	90.4	71.1	26.3
Drift Wall Crown	62.5	57.0	84.8	89.6	89.9	70.9	26.2
Drift Wall 1:30	62.6	57.1	84.9	89.6	89.9	70.9	26.2
Drift Wall Rib	62.6	57.0	84.8	89.6	89.9	70.9	26.3
Drift Wall 4:30	62.3	56.8	84.6	89.5	89.8	70.8	26.3
Invert Top-Center	68.8	60.7	87.0	91.1	91.1	71.4	26.3
Invert Top-Right	63.3	57.5	85.1	89.8	90.0	70.9	26.3
Cool WP (DHLW)							
Waste Pkg Upper Half	62.9	57.9	85.3	90.0	90.2	71.0	26.3
Waste Pkg Lower Half	63.2	58.1	85.5	90.1	90.3	71.1	26.3
Drip Shield Top-Center	61.9	57.4	85.1	89.8	90.1	71.0	26.3
Drip Shield Top-Corner	61.7	57.3	85.0	89.7	90.0	70.9	26.3
Drip Shield Bottom-Corner	61.5	57.1	84.9	89.7	90.0	70.9	26.3
Drift Wall Crown	60.0	56.2	84.3	89.3	89.6	70.8	26.2
Drift Wall 1:30	60.1	56.2	84.4	89.3	89.7	70.8	26.2
Drift Wall Rib	59.9	56.1	84.3	89.2	89.6	70.8	26.2
Drift Wall 4:30	59.5	55.8	84.1	89.1	89.5	70.7	26.3
Invert Top-Center	63.1	58.1	85.5	90.1	90.3	71.1	26.3
Invert Top-Right	60.3	56.4	84.4	89.3	89.7	70.8	26.3

Source: Produced using files from Buscheck 2001 [DIRS 155243].

NOTE: * = Time of Preclosure Peak T
** = Time of Postclosure Peak T
*** = Near-Ambient T.

Table 5.4-1. Sequence of Steps to Combine Submodel Results in the Multiscale Thermal-Hydrologic Model (Page 1 of 2)

Step	Dimensionality	Physical Processes	Physical Domain	Heat Source	Boundary Conditions	Number of Submodel Runs
1. Smeared-heat-source mountain-scale thermal **(SMT) submodel.**						
	3D	Conduction only, vertical property variation	Repository footprint plus >0.7 km edges, surface to 1 km below water table	Smeared, 1-m thick, within footprint, reduced during ventilation	No heat flow at sides, constant temperature at bottom and surface	1
2. Smeared-heat-source drift-scale thermal **(SDT) submodel.** At 33 selected columns. Run at 4 AMLs bracketing the actual AML						
	1D	Conduction only in rock, vertical property variation, radiation in drift, approximated natural convection	Surface to water table	Smeared, 1-m thick, reduced during ventilation	Constant temperature at surface, constant temperature at water table	4x33=132
3. **Interpolate** results at each column and time step to additional locations within the footprint. HTOM: 671 locations, LTOM: 762 locations						
4. At each location and selected time steps, determine the interpolated AML in the SDT array to match the local SMT temperature. **Result**: At each location and time step there is an effective repository horizon AML that represents the effectiveness of the heat sink volume in removing heat from the drift. An ERHAML less than the true AML indicates 3D mountain-scale heat flow.						
5. Line-heat-source drift-scale thermal-hydrologic **(LDTH) submodel.** At the same columns as in the SDT submodels. Run at 4 drift spacings creating AMLs bracketing the actual AML						
	2D	Heat and mass transfer, vertical property variation, radiation in drift, approximated natural convection	Mid-drift to mid-pillar, surface to water table	Waste package volume-preclosure, volume under drip shield-postclosure, line-averaged, reduced during ventilation	No heat or mass flow at sides, constant temperature, pressure, and relative humidity at surface, imposed water flux map at surface, constant temperature, pressure, and saturation at water table	4x33=132

Table 5.4-1. Sequence of Steps to Combine Submodel Results in the Multiscale Thermal-Hydrologic Model (Page 2 of 2)

<table>
<tr><th>Step</th><th>Dimensionality</th><th>Physical Processes</th><th>Physical Domain</th><th>Heat Source</th><th>Boundary Conditions</th><th>Number of Submodel Runs</th></tr>
<tr><td colspan="7">6. Interpolate temperatures at each zone and time step to additional locations within the footprint.
HTOM: 671 locations, LTOM: 762 locations</td></tr>
<tr><td colspan="7">7. At each of the locations and selected time steps, use the effective ERHAML (from Step 4) to interpolate among the AMLs
Result: Temperatures at 671 or 762 locations (higher- or lower-temperature operating mode), consistent with edge effects, infiltration map and drift layout, but not including three-dimensional WP-to-WP variations. These are termed line-source, mountain-scale thermal-hydrologic (LMTH) temperatures.</td></tr>
<tr><td colspan="7">8. Discrete-heat-source drift-scale thermal (DDT) submodel
At one location.
Run at same AMLs as SDT and LDTH submodels.</td></tr>
<tr><td></td><td>3D</td><td>Conduction only in rock, vertical property variation, radiation in drift, radiation under drip shield, no natural convection</td><td>Mid-drift to mid-pillar, surface to water table, No drip shield during preclosure</td><td>Eight full and two half WPs (of same diameter, but individual lengths and thermal powers), reduced during ventilation</td><td>No heat flow at sides, constant temperature at bottom, constant temperature at surface</td><td>4</td></tr>
<tr><td colspan="7">9. For each AML, at selected positions in each cross-section (perpendicular to the drift axis), and at selected times, the temperatures are averaged along the axial direction.
The HTOM has 28 axial positions (each WP mid-length and end). The lower-temperature operating mode has 36 positions, including two in each of the four non-minimum gaps</td></tr>
<tr><td colspan="7">10. For each AML, at each WP mid-length, and at the selected times and positions in each cross-section, the WP-specific axial deviation is calculated (local temperature minus average temperature from Step 9)</td></tr>
<tr><td colspan="7">11. The location-specific (in the footprint) ERHAML is used to interpolate among the four axial deviation histories (for the selected cross-sectional positions, selected times, and selected axial positions). These deviation histories are used to adjust the LMTH temperatures from Step 7, producing discrete-source, mountain-scale, thermal-hydrologic (DMTH) temperature histories at all locations and positions within locations
Result: Temperatures across the entire domain and time history</td></tr>
<tr><td colspan="7">12. At each location, and at selected cross-sectional and axial positions, and at selected times, the WP-specific temperatures (DMTH) are compared to the four (AML-based) LDTH temperatures from Step 6 to develop a new set of Effective WP AMLs. These effective AMLs take into account axial in-drift geometry and WP power variability in addition to repository edge effects, the infiltration map, and the layout of drifts.</td></tr>
<tr><td colspan="7">13. At each location, and at selected cross-sectional and axial positions, and at selected times, the Effective WP AMLs are used to interpolate on the four (AML-based) LDTH sets of (non-temperature) parameters.
Result: All non-temperature variables across the entire domain and time history</td></tr>
</table>

Source: Produced from information in CRWMS M&O 2000 [DIRS 149862].

NOTES: Selected times and positions refer to positions and times used in downstream models.
AML = areal mass loading; WP = waste package.

Table 5.4.3-1. Sensitivity of In-Drift Thermal-Hydrologic Performance to Uncertainties and Parameters (Page 1 of 3)

Section	Parameter or Uncertainty	Range of Parameter or Uncertainty	Base Case	Performance Measure	Effect of Parameter or Uncertainty Range on Performance Measure
5.3.1.4.1	Gas storage in lithophysal cavities	Include or Exclude	Exclude	Fraction of vaporizing liquid included in model	0.1% over-estimate of volume of vaporized liquid displaced to adjacent zones
5.3.1.4.2 HTOM, LTOM	Fracture heterogeneity aspects of seepage	Include or Exclude	Exclude	Seepage flux-, DW T & RH; DS T & RH	Increases likelihood of seepage during the sub-boiling period
5.3.1.4.3	Imbibition hysteresis	Include or Exclude	Exclude	DW & DS T&RH	Non-conservatively bounded T (under predict) Conservatively bounded RH (over-predict)
5.3.1.4.4 HTOM, LTOM	Buoyant gas-phase convection (drift-)	± 2 standard deviations k_b = 0.15 – 38 Darcy, Half-pillar scale	k_b = 2.4	Percolation flux, DW & DS T	HTOM boiling period: up to double the heat-mobilized liquid-phase flux; peak temperature range of 11°C; boiling period range of 50 years
5.3.1.4.5	THC processes	Include or Exclude	Exclude	change in bulk permeability (k_b)	Changes within natural variation of k_b
5.3.1.4.6 HTOM	THM processes	Include or Exclude	Exclude	change in bulk permeability (k_b)	>5 orders magnitude decrease k_b during thermal period, 6x permanent increase in k_b (within range of k_b variability)
5.3.1.4.7 HTOM, LTOM	Host rock permeability	k_b = 0.15 — 38 Darcy	Mean k_b (unit dependent) K_b = 2.38	DW T & RH, DS T & RH, INV_U S	DW T 11°C
5.3.1.4.8 HTOM, LTOM	Host rock thermal conductivity	K_{th} = 1.13-2.02 wet K_{th} = 0.64-1.54 dry	Mean: 1.87 wet; 1.27 dry	DW T & RH, DS T & RH, INV_U S	DW & DS T ~85°C range, HTOM; DW & DS T ~20°C range, LTOM
5.3.1.4.9 HTOM, LTOM	Lithophysal porosity (combined influence on thermal conductivity and heat capacity)	0 to 25%	Mean porosity: 12.5%	DW T & RH, DS T & RH, INV_U S	DW & DS T ~100°C range, HTOM; DW & DS T ~25°C range, LTOM

Table 5.4.3-1. Sensitivity of In-Drift Thermal-Hydrologic Performance to Uncertainties and Parameters (Page 2 of 3)

Section	Parameter or Uncertainty	Range of Parameter or Uncertainty	Base Case	Performance Measure	Effect of Parameter or Uncertainty Range on Performance Measure
5.3.1.4.10 LTOM	Invert thermal conductivity	0.15 to 3.04	0.15	DW T & S, DS T & RH, INV_L T & S	DW & DS 2-4°C range, INV_L 9°C range, INV S 5-9% after rewetting
5.3.1.4.11 LTOM	WP capacity drift spacing WP spacing	16-21 PWR SNFAs 81-97 m drift spacing 0.1-2 m average WP spacing	21 SNFAs, 81 m drift spacing 0.1 m WP spacing	Peak WP T	3°C range
5.3.2.4.1 HTOM	Ventilation Efficiency, HTOM	ANSYS, MULTIFLUX, Quarter-Scale Test	ANSYS	15 m^3/s Average Efficiency, 50 yrs (or scaled values)	ANSYS 74%, MULTIFLUX 94%, Test 83%
5.3.2.4.2 HTOM, LTOM	Ventilation Efficiency	±10%	70% HTOM, 80% LTOM	DS T postclosure peak	HTOM 14°C range, LTOM 7°C range
5.3.2.4.2 HTOM, LTOM	Ventilation efficiency time dependence	Constant or time-dependent	Constant	DS T preclosure peak	HTOM 59°C range, LTOM 63°C range
5.3.2.4.3 LTOM	Ventilation Duration	±22 years	300 years	LTOM DS T postclosure peak	3°C range
5.3.2.4.4 HTOM, LTOM	Water entering drift	6 months to dryout 3 m rock, 10 mm/yr flux entering from 11.5 m wide region; Calculated dryout	No water entering drift	RH at 500 m in ventilation air, kW/m latent heat removal, DS T postclosure	9.9% no water entry, 33% during dry out, 10.1% after dry out; 1.29 kW/m during dry out, <0.01 kW/m after dryout; Negligible T effect
5.3.2.4.4 HTOM	In-drift seepage, and NF dry out due to ventilation	0-30% percolation flux seepage	0% seepage	DS T postclosure	Negligible effect
5.3.2.4.5 HTOM, LTOM	Treatment of thermal radiation	Correlation-based or explicit	Explicit	Peak DS T	6°C range (HTOM)

Table 5.4.3-1. Sensitivity of In-Drift Thermal-Hydrologic Performance to Uncertainties and Parameters (Page 3 of 3)

Section	Parameter or Uncertainty	Range of Parameter or Uncertainty	Base Case	Performance Measure	Effect of Parameter or Uncertainty Range on Performance Measure
5.3.2.4.5	Treatment of natural convection heat transfer	Correlation-based or Navier-Stokes CFD	Correlation-based	DS and WP T	Can match perimeter-average T, with CFD-based correlation; details along perimeter can affect condensation locations
5.3.2.4.5 HTOM	Treatment of natural convection mass transfer	0 to 2×10^{-5} m^2 in-drift bulk permeability	10^{-8} m^2	DW T & S, DS T & RH, INV_L T & S	INV_L/DW & DS 2-4°C range, INV_L S minor changes during re-wetting
5.3.2.4.6 HTOM, LTOM	3D in-drift effects	2D versus 3D	3D	WP T (DB, AVG, COOL) postclosure peak	HTOM 26°C range, LTOM 8°C range

Source: Produced from results in Sections 5.3.1.4 and 5.3.2.4 of this document.

NOTES: 2D = two-dimensional; 3D = three-dimensional; CFD = computational fluid dynamics; DS = drip shield; DW = drift wall; HTOM = higher-temperature operating mode; INV_L = lower-center of invert; INV_U = upper layer of invert just outboard of the drip shield; LTOM = lower-temperature operating mode; NF = near-field; PWR = pressurized water reactor; RH = relative humidity; S = saturation; SNFA = spent nuclear fuel assembly; T = temperature; WP = waste package.

DB, AVG, COOL (WP) = Design Basis (11.8 kW initial), Average (7.4 kW average BWR), Cool (DOE high-level waste glass), 0.3 kW waste packages.

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