4. SEEPAGE

4.1 INTRODUCTION AND CONCEPTUAL BASIS

Seepage of water into waste emplacement drifts is considered one of the principal factors having the greatest impact on the long-term safety of the repository system (CRWMS M&O 2000 [DIRS 148713], Volume II, Table 4-1). The number of waste packages contacted by water, the corrosion rate of engineered barriers and waste packages, the dissolution and mobilization of radionuclides, and the release and migration of radionuclides to the accessible environment all depend on the rate, chemical composition, and spatial and temporal distribution of water seeping into the emplacement drifts.

This section summarizes process modeling and uncertainty studies performed to estimate seepage of liquid water into emplacement drifts as shown in Table 4-1. The initial issues of the seepage-related analysis model reports (AMRs) supported the *Total System Performance Assessment for the Site Recommendation* (TSPA-SR) (CRWMS M&O 2000 [DIRS 153246]). Additional studies and sensitivity analyses were conducted to address the following specific uncertainty issues:

- Data from long-term liquid-release experiments were analyzed to reduce the estimation uncertainty of seepage–relevant parameters and obtain estimates for the previously untested lower lithophysal zone of the Topopah Spring Tuff unit. The related modeling activity is fully documented in the *Seepage Calibration Model and Seepage Testing Data* (CRWMS M&O 2001 [DIRS 153045]). As a consequence of the new calibration results, the seepage model for *Total System Performance Assessment* (TSPA) was also updated, as documented in *Seepage Model for PA Including Drift Collapse* (CRWMS M&O 2000 [DIRS 153314]). Finally, the seepage abstraction was revised to reflect the reduced uncertainties (CRWMS M&O 2001 [DIRS 154291]). All these studies are concerned with seepage under ambient temperature conditions. The results of these activities were not included in the TSPA-SR; they are summarized in Section 4.3.1.

- Distributions of flow focusing factors were developed as part of the seepage abstraction process to account for potentially increased local flow rates as a result of intermediate-scale flow channeling. A conservative flow focusing model was applied in *Abstraction of Drift Seepage* (CRWMS M&O 2001 [DIRS 154291], Section 6.4.3). To better quantify flow focusing and to address the uncertainty associated with the estimation of flow focusing factors, a detailed process model was developed to simulate water flow through a stochastically generated, heterogeneous fracture continuum. The results of this study, which did not support the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) and which do not consider elevated temperature conditions, are reported in Section 4.3.2.

- Seep flow rates were increased by a safety factor to account for the potential impact of rock bolts on seepage (CRWMS M&O 2001 [DIRS 154291], Section 6.4.1). A detailed modeling study was performed to address the potential for seepage enhancement due to ground support measures, and thus the necessity of this safety factor. This study, the

Table 4-1. 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			Section of Volume 1	Performance Assessment Treatment of Supplemental Scientific Model or Analysis[a]	
			Unquantified Uncertainty Analysis	**Update in Scientific Information**	**Lower-Temperature Operating Mode Analysis**		**TSPA Sensitivity Analysis**	**Included in Supplemental TSPA Model**
Limited Water Entering Emplacement Drifts	Seepage into Emplacement Drifts (4.2.1)	Flow-focussing within heterogeneous permeability field; episodic seepage	X		X	4.3.1 4.3.2 4.3.5	X	X
		Effects rock bolts and drift degradation on seepage	X			4.3.3 4.3.4		
	Coupled Effects on Seepage (4.2.2)	Thermal effects on seepage	X		X	4.3.5	X	X
		Thermal-Hydrologic-Chemical effects on seepage	X		X	4.3.6		
		Thermal-Hydrologic-Mechanical effects on seepage		X	X	4.3.7		

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]).

results of which were not included in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]), is described in Section 4.3.3.

- Seepage is also potentially increased by a change in the drift geometry due to rockfall and drift degradation. A simplified, two-dimensional drift-degradation model supported the seepage calculations that were used for the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]). A new seepage prediction model based on three-dimensional degradation profiles was developed to further study the impact of heterogeneity and degradation effects on seepage. This study, documented in Section 4.3.4, did not include thermal loading scenarios and was not used to support the TSPA-SR.

- In the studies supporting the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]), effects of repository heat on seepage were deduced indirectly from results presented in *Mountain-Scale Coupled Processes (TH) Models* (CRWMS M&O 2000 [DIRS 144454]). A refined modeling study was performed to reduce conceptual uncertainties regarding grid resolution and heterogeneity. The study also examined the impact of lithophysal cavities on thermal properties; the potential for liquid water to penetrate a superheated region, causing episodic seepage events; and the development of a vaporization barrier. Moreover, percolation flux was calculated for a range of thermal operating modes. The new simulation work is presented in Section 4.3.5; it was not considered in the TSPA-SR.

- Thermal-hydrologic-chemical (THC) processes may impact seepage through thermally induced changes in unsaturated hydrogeologic properties. The TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) was based on an abstraction of the data documented in *Drift-Scale Coupled Processes (DST and THC Seepage) Models* (CRWMS M&O 2000 [DIRS 142022]). Additional validation studies were performed, enhancing the confidence in the THC modeling approach. Sensitivity analyses were performed to examine different in-drift designs, different heterogeneous host rock units, different systems of components and minerals, different kinetic models for mineral-water interactions, different permeability-porosity relations during precipitation and dissolution, and changed thermodynamic data and initial conditions. All these studies, which are fully documented in *Drift-Scale Coupled Processes (DST and THC Seepage) Models* (BSC 2001 [DIRS 154677]), helped reduce conceptual uncertainties in the THC models. Additional studies of coupled processes were performed for an extended range of temperatures covering various thermal operating modes. All these studies are summarized in Section 4.3.6.

- A distinct-element analysis was performed to examine thermal-mechanical (TM) effects of drift excavation and repository heat on hydrogeological properties (CRWMS M&O 2000 [DIRS 149040]). This analysis has been revised and extended to provide a more robust estimate of TM effects in fracture permeability. In addition, a fully coupled thermal-hydrologic-mechanical (THM) continuum model was developed and calibrated against air-permeability data from three niches and the Drift Scale Test area. The successful calibration increased confidence in the conceptual model and reduced uncertainties in the subsequent prediction runs, which included two thermal operating modes. This study is presented in Section 4.3.7.

All the following sections discuss calculations done before the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]), as documented in AMRs, and the calculations done after the TSPA-SR, as documented in updates to the AMRs and this report. Each section contains a discussion of independent evidence from analogue sites. In addition, the remaining unquantified uncertainties are identified and summarized.

Like any other model, seepage models are simplifications and abstractions of recognized processes and features. These processes and features were included in a specific seepage model based on their expected significance, which can be evaluated through sensitivity analyses. Experiments were designed and conducted to identify, understand, and characterize significant processes and parameters. Remaining uncertainties and property variabilities were considered either by stochastic simulations and uncertainty propagation analyses or by modeling appropriately increased parameter uncertainties in the TSPA calculations. Conservative approaches were used for effects that could not be explicitly accounted for because the amount, type, or quality of characterization data was insufficient.

Any remaining uncertainty is only of concern if it affects the goal of the respective study. Conversely, even a small, well-understood, and accurately quantified uncertainty may be unacceptable if the outcome of an analysis is very sensitive to a change in the corresponding conceptual model, its data, or parameter values. The following discussion therefore includes both quantified and unquantified uncertainties.

4.2 TREATMENT OF SEEPAGE-RELATED ISSUES

Figure 4.2-1 illustrates some seepage-relevant phenomena and processes. The following paragraphs discuss the key factors affecting drift seepage and how they were addressed in the reports listed in Section 4.1. As mentioned above, some of these reports were revised and finalized after the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]). Note, however, that the general modeling approach outlined here is identical to the one used for the AMRs that support the TSPA-SR. These sections represent new work and extensions of existing work. Table 4-1 identifies the primary reason for the development of each section and indicates which of these analyses have been included in TSPA calculations.

4.2.1 Spatial and Temporal Flow Focusing

Process Description–Flux and spatial distribution of downward percolating water is one of the most important factors affecting seepage rates and seep locations. Water movement is controlled by net infiltration at the surface and subsequent multiscale moisture redistribution. Hydrostratigraphic units (such as the PTn) and features (such as faults) govern large-scale flow patterns, and thus lead to a redistribution of infiltration and percolation fluxes. On an intermediate scale, flow through the fracture network may be focused (funneling effect) or dispersed (bifurcation). This leads to zones of locally higher percolation fluxes and areas of reduced water flow between them. Water within such a high-flux zone may be further channeled by variabilities in the fracture network. Finally, heterogeneity and flow instabilities within individual fractures lead to small-scale flow channels (rivulets or fingers). In addition to spatial flow focusing, episodic events may lead to temporally increased percolation fluxes, followed by periods of reduced percolation. This phenomenon can be referred to as temporal flow focusing (analogous to spatial flow focusing).

Current Modeling Approach and Uncertainties–Uncertainties in the spatial and temporal distribution of percolation flux encountering the emplacement drifts were addressed on the different scales (i.e., mountain scale, intermediate scale, drift scale, sub-drift scale) and were propagated through the downstream models using deterministic sensitivity analyses (CRWMS M&O 2000 [DIRS 122797], Section 6.6), probabilistic flow focusing factors (CRWMS M&O 2001 [DIRS 154291], Section 6.3.3), and an estimation of effective seepage-relevant parameters (CRWMS M&O 2001 [DIRS 153045], Section 6.3.3 and 6.4.3).

4.2.2 Capillary Barrier Effect

Process Description–Under unsaturated conditions, the rate of water dripping into the opening is expected to be less than the downward percolation rate because the cavity acts as a capillary barrier (Philip et al. 1989 [DIRS 105743], pp. 16 to 28). If percolating water encounters the cavity, the relatively strong capillary forces in the geologic formation retain the water, preventing it from seeping into the drift. Water accumulates at the drift ceiling, where the increase in saturation leads to capillary pressures that are locally less negative than in the surrounding rock, allowing water to be diverted around the drift. If the lateral hydraulic conductivity is insufficient to divert all the water, seepage is initiated; the corresponding flux is referred to as the "seepage threshold." The effectiveness of the capillary barrier is determined by the capillarity, as well as the permeability and connectivity of the fractures.

Current Modeling Approach and Uncertainties–The capillary barrier effect was incorporated through use of a physically based numerical model that included saturation-dependent capillary pressures and relative permeabilities. Conceptual uncertainties in fractured rock (with regard to the capillary barrier effect) were addressed by theoretical analyses (Finsterle 2000 [DIRS 151875], pp. 2055 to 2066); direct observations during the seepage field tests (CRWMS M&O 2000 [DIRS 141400], Section 6.2); calibration of the model against seepage-relevant data, followed by model validation exercises (CRWMS M&O 2001 [DIRS 153045], Section 6.3.4 and 6.4.4); and analogue studies (see Section 4.3.1.7). Remaining uncertainties regarding the location-specific effectiveness of the capillary barrier are being addressed by performing additional seepage tests under controlled humidity conditions (see Section 4.3.1.5).

4.2.3 Excavation-Disturbed Zone

Process Description–The properties of the fractured rock in the immediate vicinity of the drift wall control the capillary barrier effect, which occurs within a relatively small region around the opening. The thickness of this boundary layer is approximately given by the height to which water rises on account of capillarity, and it is likely to be smaller than the extent of the zone affected by excavation-induced stress redistribution and related rock deformations (e.g., opening and closing of existing fractures, generation of new microfractures and cracks) (Wang and Elsworth 1999 [DIRS 104366], pp. 751 to 757).

Current Modeling Approach and Uncertainties–The seepage-relevant properties of the region affected by the capillary barrier were determined by calibration against liquid release test data.

As a result of the calibration approach used, the potential impact of the excavation-disturbed zone on seepage was automatically considered, effectively eliminating potential conceptual and parametric errors in a modeling approach that requires the development of a hydromechanical model. Additional effects and uncertainties are discussed in Section 4.3.7.

4.2.4 Drift Geometry and Drift Surface Effects

Process Description–The geometry (i.e., the shape and size) of the emplacement drift determines the likelihood of encountering seeps and the ease with which water can be diverted around the opening. The geometry of drift wall roughness and the characteristics of the drift surface (e.g., wettability, micro-roughness, dust, coating) partially control local water accumulation, droplet formation, the potential for film flow along the drift wall, and, eventually, dripping locations. The frequency, location, size, and geometry of breakouts and partial drift collapse affect the integrity of the capillary barrier. Breakouts may lead to distinct topographic lows, which increase seepage, or a more cone-shaped drift, which would promote flow diversion and decrease seepage.

Current Modeling Approach and Uncertainties–Simulations of seepage into drifts with cavities extending from the drift surface were conducted to examine the impact of rockfall on seepage rates (CRWMS M&O 2000 [DIRS 153314], Section 6.4). Rock bolts were treated in a conservative manner by forcing water flowing in the vicinity of a rock bolt to seep (CRWMS M&O 2000 [DIRS 153314], Section 6.7). Detailed submodels on the significance of the presence of rock bolts for ground support and drift degradation are presented in Sections 4.3.3 and 4.3.4, respectively.

4.2.5 Ventilation and Evaporation-Condensation Effects

Process Description–The drift temperature, drift humidity, and regulation of temperature and humidity in the drift by ventilation determine evaporation and condensation effects. Evaporation at the drift wall generally reduces drop formation and dripping, and creates a dryout zone around the drift. If relative humidity in the drift is kept below 100 percent by ventilation, then seepage of liquid water is reduced or completely suppressed. However, local differences or temporal changes in drift temperature may lead to condensation of vapor, causing droplet formation at the drift wall and other surfaces within the drift. Accumulation of condensate can lead to dripping.

Current Modeling Approach and Uncertainties–Ventilation effects were not explicitly modeled. Neglecting ventilation effects in a seepage prediction model is a conservative approach: such calculations lead to increased seepage because water that potentially evaporates is considered to be dripping into the opening, enhancing the seepage rate. However, if significant evaporation occurred during the seepage experiments, then the parameter estimates obtained by calibration would be nonconservative (see Section 4.3.1.8). Uncertainties regarding evaporation effects were addressed by selecting conservative parameter sets in the seepage abstraction (CRWMS M&O 2001 [DIRS 154291], Section 6.3 and 6.4). In-drift moisture migration and condensation are separate issues (see Section 5).

4.2.6 Thermal Effects and Coupled Processes

Process Description–Repository heat may impact seepage through coupled thermal-hydrologic-chemical-mechanical effects on rock properties or through the redistribution of water around the drifts and the development of a vaporization barrier. Thermal expansion, as well as dissolution and precipitation of minerals, leads to changes in fracture aperture and fracture coatings, potentially affecting unsaturated zone (UZ) hydrogeologic properties and fracture-matrix interaction. Vaporization and recondensation leads to pressure changes and redistribution of water and heat. A vaporization barrier may prevent percolation water from reaching the drifts. The chemistry of the seepage water may be affected by thermally induced changes in the thermodynamic and geochemical environment.

Current Modeling Approach and Uncertainties–The thermal effects on the hydrologic, mechanical, and chemical processes are examined through coupled process models, as described in Sections 4.3.5 through 4.3.7. Uncertainties in these models stem mainly from uncertainties in the coupling terms and additional parameters that have to be specified. These conceptual and parametric uncertainties are examined through extensive sensitivity analyses. In general, however, these coupled models are used to support the simplifying or conservative approaches used during seepage abstraction.

4.3 DISCUSSION OF KEY PROCESSES, MODELS, AND RELATED UNCERTAINTIES

4.3.1 General Seepage Evaluation and Estimation of Seepage-Relevant Parameters

4.3.1.1 Introduction

This section summarizes the modeling and uncertainty studies performed to determine the seepage-relevant hydrogeologic parameters of the geologic formation in which the potential repository will be sited. Air-permeability and short-term seepage data from liquid-release tests conducted in Exploratory Studies Facility (ESF) Niche 2 (Station 36+50) were used to develop and calibrate a model (the seepage calibration model) for the estimation of seepage-related parameters. This model, along with the related seepage model for performance assessment and the corresponding seepage abstraction, was documented in *Seepage Calibration Model and Seepage Testing Data* (CRWMS M&O 2000 [DIRS 119412]), *Seepage Model for PA Including Drift Collapse* (CRWMS M&O 2000 [DIRS 122894]), and *Abstraction of Drift Seepage* (CRWMS M&O 2000 [DIRS 142004]). The results from these three reports (which are briefly summarized in Section 4.3.1.3) support the TSPA-SR evaluation of seepage fraction and seep flow rate (CRWMS M&O 2000 [DIRS 153246], Section 3.2.4).

New air-permeability and long-term, near-steady seepage data from liquid-release tests conducted in ESF Niches 3 (Station 31+07) and 4 (Station 47+88), as well as borehole SYBT-ECRB-LA#2, were used to extend the model and reduce the uncertainty in the estimated parameters (CRWMS M&O 2001 [DIRS 153045], Section 6). The seepage model for performance assessment and related seepage abstraction have been updated accordingly, as documented in *Seepage Model for PA Including Drift Collapse* (CRWMS M&O 2000 [DIRS 153314]) and *Abstraction of Drift Seepage* (CRWMS M&O 2001 [DIRS 154291]), respectively. These three AMRs are summarized in Sections 4.3.1.4 and 4.3.1.6. The new results were not available in time to be used for the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]). However, they are consistent with and therefore support the previous findings that were used for TSPA-SR (CRWMS M&O 2000 [DIRS 153426]). A short description of this additional seepage testing is provided in Section 4.3.1.5.

Uncertainties with respect to specific seepage-related issues (such as flow focusing, rock bolts, drift degradation, and the impact of thermal, chemical, and mechanical effects on seepage) are presented in Sections 4.3.2 to 4.3.7. The method used to determine seepage-relevant properties consists of a combination of field testing, process modeling, and effective parameter estimating. This approach was chosen because it provides the means to test the appropriateness of the conceptual model, to reduce and quantify parametric uncertainties, and to obtain seepage-relevant, model-related parameters suitable for use in drift-scale seepage prediction models. Random errors in the field data used for model calibration were accounted for in the calculation of the parameter estimation uncertainties, which in turn were propagated through the seepage model for performance assessment (CRWMS M&O 2000 [DIRS 153314]) to arrive at uncertainty ranges for use in the subsequent seepage abstraction (CRWMS M&O 2001 [DIRS 154291]). Remaining unquantified uncertainties (specifically regarding spatial variability of seepage-relevant rock properties, local percolation flux distribution, and the impact of design decisions regarding ventilation, thermal loading, repository extent, and drift orientation) were addressed through appropriately broadened uncertainty distributions and conservative modeling in the abstraction (CRWMS M&O 2001 [DIRS 154291], Sections 5, 6.3, and 6.4; see also Sections 4.3.2 to 4.3.7). Unquantified conceptual uncertainties were assessed in analogue studies and other corroborating observations.

4.3.1.2 Goal of Models

The goals of the models used to derive seepage-relevant parameters and examine seepage behavior—the seepage calibration model (CRWMS M&O 2001 [DIRS 153045]), the seepage model for performance assessment (CRWMS M&O 2000 [DIRS 153314]), and the abstraction of drift seepage (CRWMS M&O 2001 [DIRS 154291])—are:

- Provide a methodological and conceptual basis for the development of seepage prediction models
- Derive seepage-relevant parameters
- Identify conceptual uncertainties and estimate uncertainty and variability of seepage-relevant parameters
- Determine the seepage rate, its variability, and its uncertainty.

The seepage models were intended to provide estimates of the seepage flux averaged over a 5-m drift segment (the approximate length of a waste package) as a function of the percolation flux on the drift scale. Consequently, the seepage models were not expected to accurately predict individual seepage events or the precise spatial distribution along the emplacement drift axis or the drift ceiling. Instead, average seepage rates were calculated for a drift segment, which is the scale of interest.

Once seepage rates were evaluated deterministically for a wide range of conditions (which was the purpose of the seepage model for performance assessment), a probabilistic analysis was performed to include uncertainty and spatial variability in TSPA calculations.

4.3.1.3 Discussion of Results

The development of a conceptual seepage model was guided by the recognition that the seepage process in a fractured porous medium is too complex to warrant the construction of a detailed process model. Such a model would consist of a deterministic calculation of unsaturated water flow through a fracture network, which would have to include multiscale variabilities in hydraulic properties. The necessary characterization data are not available, and it is not feasible to obtain them in full. A key element of the chosen approach was therefore the reliance on inverse modeling and the estimation of seepage-relevant, model-related parameters. This approach was considered appropriate because:

- A detailed simulation of individual seeps is not necessary for the intended use of the model: estimating average seepage rates into emplacement drifts.
- Certain factors affecting seepage can be combined into effective parameters; estimating effective parameters partly compensates for processes and features not explicitly considered in the model.
- Calibrating a model against data from seepage experiments ensures the model captures the relevant processes.
- The estimated parameters can be considered optimal and used directly in the prediction model.
- The relative simplicity of a calibrated continuum model leads to less uncertainty in subsequent seepage predictions.

The development of the seepage calibration model is documented in *Seepage Calibration Model and Seepage Testing Data* (CRWMS M&O 2000 [DIRS 119412]). A geostatistical analysis of post-excavation air-permeability data provided the basis for generating a heterogeneous property field, which was mapped onto the model grid. Short-term liquid-release tests from ESF Niche 2 (Station 36+50, located in the middle nonlithophysal zone of the Topopah Spring welded unit [Tptpmn]) were simulated, and the model was calibrated against a relatively small set of cumulative seepage data. The calibrated model was then tested using data from additional liquid-release experiments from Niche 2. Based on the same conceptual model, an extensive sensitivity analysis was performed, using the seepage model for performance assessment (CRWMS M&O 2000 [DIRS 122894]) to derive a database of seepage rates to be used in the subsequent seepage abstraction (CRWMS M&O 2000 [DIRS 142004]), in which probability density functions for seepage rate and seepage fraction were developed.

These results were considered in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246], Section 3.2.4). However, the sensitivity and error analyses revealed strong correlations and relatively large uncertainties in the estimated parameters, mainly because the amount of water used in the short-term liquid-release tests was insufficient (CRWMS M&O 2000 [DIRS 119412], Section 6.4). Additional, longer-term liquid-release tests were needed to reduce the estimation uncertainty, to better evaluate the spatial variability of seepage, and to obtain seepage data from the lower lithophysal zone of the Topopah Spring unit (Tptpll). New seepage tests were conducted, and the affected documents were revised (see Section 4.3.1.4).

4.3.1.4 Discussion of Revision 01 Results

The revised seepage studies were based on the general modeling approach outlined in *Seepage Calibration Model and Seepage Testing Data* (CRWMS M&O 2000 [DIRS 119412]). However, they incorporated the new data that became available for model calibration. The analyzed data included more than 200 air permeabilities, as well as seepage rates from approximately 60 liquid-release tests conducted at three niche sites along the ESF (Niches 3 [Station 31+07], 2 [Station 36+50], and 4 [Station 47+88]) and in Enhanced Characterization of the Repository Block (ECRB) Cross Drift borehole SYBT-ECRB-LA#2, located in the Tptpll unit (CRWMS M&O 2001 [DIRS 153045]).

Figure 4.3.1-1 shows an example of a three-dimensional, heterogeneous model used to determine seepage-relevant, model-related parameters through calibration against seepage rate data obtained on the drift scale. Details about the calibration process can be found in *Seepage Calibration Model and Seepage Testing Data* (CRWMS M&O 2001 [DIRS 153045], Sections 6.3.3 and 6.4.3). The calibrated model was able to predict seepage rate data from other long-term liquid-release tests reasonably well, especially when considering the prediction uncertainty (CRWMS M&O 2001 [DIRS 153045], Sections 6.3.4 and 6.4.4; see also Figure 4.3.1-2). The resulting estimates for permeabilities and the van Genuchten capillary strength parameter, $1/\alpha$, were used in the seepage model for performance assessment to calculate seepage thresholds and seepage rates as a function of percolation flux, as described in *Seepage Model for PA Including Drift Collapse* (CRWMS M&O 2000 [DIRS 153314], Section 6.6). That document also describes additional sensitivity analyses regarding parameters of secondary importance (such as the van Genuchten parameter n, the standard deviation and correlation length of the permeability field), certain conceptual model features (such as the correlation between permeability and the van Genuchten capillary strength parameter, $1/\alpha$, the stochastic realization of the permeability field), and the impact of rock bolts and drift degradation on seepage.

The calibration and validation studies presented in *Seepage Calibration Model and Seepage Testing Data* (CRWMS M&O 2001 [DIRS 153045], Section 6) were not reflected in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]). However, they are consistent with and support the AMRs used for the TSPA-SR. In addition, they addressed some of the uncertainty issues related to seepage, specifically:

- The conceptual model and its numerical implementation proved adequate for the simulation and reproduction of average drift-scale seepage behavior in a fractured rock.

- Parameters were derived (specifically the van Genuchten capillary strength parameter, $1/\alpha$) that are relevant for seepage on the scale of interest. Parameters determined through calibration are suitable for use in the numerical seepage prediction model and its submodels, which were developed for sensitivity analyses.

- Estimation uncertainties were determined using conventional linear error analysis, which accounts for the goodness-of-fit and the sensitivity of the simulated data to the parameter of interest. Parameter values from individual borehole intervals, test locations, and hydrogeologic units were averaged, and measures of variability were calculated.

- Seepage rates were predicted over appropriate parameter ranges for subsequent use in seepage abstraction and probabilistic TSPA calculations.

The additional studies documented in the revised AMRs confirmed the appropriateness of the approach developed in the original AMRs. Moreover, the extended data set used for calibration and model validation reduced estimation uncertainty and increased confidence in the models. The long-term seepage experiments provided more reliable data on a larger, more relevant scale, enabling the calculation of suitable averages. Because near-steady seepage data were available, the correlation between the estimated parameters was lowered, which again reduced estimation uncertainties and the impact of potential systematic errors. Seepage data from the lower lithophysal unit were analyzed for the first time, providing unit-specific estimates. These new estimates replaced the previous conservative modeling that had been made in the seepage abstraction regarding this unit.

4.3.1.5 Developments Since Revision 01

While seepage tests in multiple locations in the Tptpmn unit are available, only a few tests were performed at a single location in the Tptpll from a borehole drilled into the ceiling of the ECRB Cross Drift. Additional seepage tests in that unit are currently being conducted as part of the Systematic Borehole Testing Program in the ECRB Cross Drift. Moreover, seepage testing in ESF Niche 5 (also located in the Tptpll) has been initiated. The results from these additional seepage tests will help develop more reliable distribution functions for seepage parameters used in TSPA calculations.

As outlined in *Seepage Calibration Model and Seepage Testing Data* (CRWMS M&O 2001 [DIRS 153045], Sections 7.4 and 7.5), evaporation losses during the liquid-release tests have been identified as a potential systematic error in the measured seepage rates, and thus in the parameters derived from these data. To address this issue, current seepage tests include measures to control relative humidity or monitor the evaporation potential. Laboratory experiments were designed to increase the understanding and quantify evaporation potentials from a fractured porous geologic formation. Modeling approaches are being explored that would account for evaporation losses. Quantifying evaporation will help diminish the potential bias in the seepage data and seepage-relevant parameters, reducing uncertainty in seepage predictions.

Additional studies and model refinement are discussed in Sections 4.3.4 to 4.3.7.

4.3.1.6 Abstraction for Total System Performance Assessment

The complex physical processes affecting drift seepage cannot be addressed comprehensively in an analytical or numerical model, mainly because it is impossible to obtain sufficient characterization data over many scales to describe all the relevant geometric features and hydrologic properties. The characterization and modeling approach focused on obtaining effective parameters based on seepage-relevant hydraulic data. The seepage model for performance assessment provided seepage estimates over a wide range of hydrologic conditions (CRWMS M&O 2001 [DIRS 153314], Section 6.6).

Finally, seepage abstraction was performed to obtain probability distributions for the fraction of waste packages encountering seepage and the seep flow rate, accounting for parameter uncertainty, spatial variability, and other effects, such as focusing (see Section 4.3.2), rock bolts (see Section 4.3.3), drift degradation (see Section 4.3.4) and coupled processes (see Sections 4.3.5 through 4.3.7).

As discussed in *Abstraction of Drift Seepage* (CRWMS M&O 2001 [DIRS 154291], Section 6.3.3), seepage is mainly a function of the geometric-mean fracture permeability and the fracture capillary-strength parameter $1/\alpha$. The effects of uncertainties in these parameters are evaluated by calculating seepage for three cases: a base case, a high-seepage case, and a low-seepage case. A triangular shape is chosen for the seepage uncertainty distributions. Table 4.3.1-1 summarizes the seepage fraction, the seepage rate, and its standard deviation at the three points defining the triangular distribution as a function of percolation flux.

Table 4.3.1-1 and the distributions for the flow-focusing factor (CRWMS M&O 2001 [DIRS 154291], Figures 5 and 6) are the final products of the seepage abstraction, which are used in TSPA simulations to estimate seepage. More details about the development of these distribution functions can be found in *Abstraction of Drift Seepage* (CRWMS M&O 2001 [DIRS 154291], Section 6).

4.3.1.7 Multiple Lines of Evidence

The conceptual understanding of drifts acting as capillary barriers, which reduce seepage in comparison to the prevalent percolation flux, is supported by direct and indirect observations in underground openings, as discussed below.

The flow model for the UZ predicts that much of the groundwater will be diverted around the emplacement drifts such that the seepage flux will be much smaller than the percolation flux. A large number of different types of analogues exist that can be used to test this conclusion. These include both natural and man-made underground openings. This section provides some examples from a variety of rock types and for a variety of climatic settings.

4.3.1.7.1 Caves

Caves provide some of the best-known and longest-term examples of seepage flux in the UZ. Most caves are located in limestone, though a few are located in lava tubes. Both rock types provide a reasonable hydrologic analogue for emplacement drifts in welded tuffs at Yucca Mountain because in all three cases (limestones, lava tubes, and welded tuffs), porosity is small and fracturing that can provide pathways for water flow is common.

Some caves are located in zones of such low percolation flux that they have little, if any, measurable seepage flux. These relatively dry caves are common throughout the southwestern United States; because of their dryness, pollen and other delicate plant and animal materials have been preserved for tens of thousands to hundreds of thousands of years (Davis 1990 [DIRS 144461]; Rogers et al. 2000 [DIRS 154320]). In fact, Davis (1990 [DIRS 144461]) notes that dryness in caves is critical to preservation of biotic remains (Davis 1990 [DIRS 144461], p. 338). That such preservation is common is supported by the fact that more than 1,000 packrat middens have been collected from caves (i.e., rock alcoves, rock crevices, and caverns) throughout arid North America (Davis 1990 [DIRS 144461], p. 341), and some of these are more than 40,000 yrs old.

Other well-known examples of preservation within caves in the UZ include hundreds of caves that contain archaeological artifacts and paintings. These are common in Europe, Africa, and India, and are reported from Asia, North America, and South America (Stuckless 2000 [DIRS 151957]). In both Europe and Africa, paintings have been dated at about 30,000 yrs. Charcoal used in paintings in the Chauvet cave in France has been dated at 32,410 to 32,340 B.C. by Chauvet et al. (1996 [DIRS 152249]). Some of the paintings in this cave show an important feature of seepage flux: some of the water that enters the cave runs down the walls rather than dripping, as modeled in the TSPA model. This evidence from analogue sites suggests that film flow along the walls is a process that may also occur in emplacement drifts, reducing the amount of water that potentially drips onto the waste packages. This effect was conservatively neglected in TSPA-SR calculations.

The caves near Altamira, Spain, are located in the UZ of a fractured limestone formation that contains clay-rich layers. These caves contain paintings that are about 14,000 yrs old. Precipitation at this site is approximately 10 times greater than at Yucca Mountain. Nevertheless, seepage rates into the caves are estimated to be less than 1 percent of the expected percolation flux (Stuckless 2000 [DIRS 151957]). Moreover, there are essentially no fluctuations in the observed seepage rates, even though the precipitation rate is not constant and the UZ is only about 7 m thick (Villar et al. 1985 [DIRS 145806]).

A similar study has been reported for Kartchner Caverns in southern Arizona. Precipitation there is approximately three times that at Yucca Mountain (Buecher 1999 [DIRS 154295]), but the climate is monsoonal and most of the precipitation occurs in just two months. The caverns are located in a limestone block with an area of approximately 350 by 550 m and are covered by approximately 10 to 65 m of limestone, cherty limestone, and cherty dolomite (Jagnow 1999 [DIRS 154296]). The caverns are cut by more than 60 faults, so fracture permeability should be large. Nonetheless, less than 2 percent of the annual precipitation reaches the caves, and nearly half of that is lost to evaporation (Buecher 1999 [DIRS 154295]).

4.3.1.7.2 Excavated Openings

Man-made underground openings include the tombs of Egypt. A total of ten tombs were visited by a project scientist in October 2000. Most of these were excavated in limestone approximately 3,500 to 3,000 yrs ago, and although the climate there is somewhat drier than at Yucca Mountain, precipitation events have been strong enough to cause mud flows within the Valley of the Kings (Weeks 1998 [DIRS 154297]). Small areas of spallation of plaster from walls and ceilings can be seen in many tombs, but evidence of dripping seems to be lacking. As with Chauvet Cave, there is occasional evidence for water flow down the wall (Figure 4.3.1-3).

Buddhist monks carved several temples into basalt flows at Ajanta, India, between the second century B.C. and the sixth century A.D. and decorated them with paintings on plastered surfaces. The climate in the area is monsoonal and the precipitation, which is more than five times that at Yucca Mountain, falls in four months (Stuckless 2000 [DIRS 151957]). Nonetheless, most of the paintings are well preserved except for small areas of spallation.

The Christians of Cappadocia, Turkey, excavated underground cities and churches during the second through eleventh centuries A.D. The geology is similar to that of southern Nevada in that the bedrock is a thick sequence of silicic volcanic rocks. Visits to the underground cities and churches produced no evidence of dripping from the ceiling, but evidence for flow down a wall was found where a fracture intersected the wall (Stuckless 2000 [DIRS 151957]). As with the Egyptian tombs and Buddhist temples, some of the church paintings showed evidence of spallation.

4.3.1.7.3 Mineral Depositions in Lithophysal Cavities

Lithophysal cavities within the Topopah Spring Tuff provide a direct record of long-term seepage within the UZ at Yucca Mountain. These originated as gas pockets within the ash-flow sheet and range in diameter from a few centimeters to a meter. Locally, between 1 and 40 percent of these cavities contain secondary minerals that record a history of water ingress. Careful dating shows that the secondary minerals developed at a fairly uniform rate during at least the last 10 million years (Neymark and Paces 2000 [DIRS 127012]). The thickness of the secondary minerals, together with the chemistry of pore waters and ages of deposition, allow calculation of a seepage rate (Marshall et al. 2000 [DIRS 151018]). The results indicate only 1 L of water per 5-m length of tunnel per year, which is significantly less than rates predicted with the seepage model for performance assessment, on the order of 10 to 1,000 L per waste package per year (CRWMS M&O 2001 [DIRS 154291], Section 6.5). Marshall et al. (2000 [DIRS 151018]) also note that no lithophysal cavities have been found that show any evidence of dripping into the cavities, such as stalactitic deposits. These findings support the concept of a capillary barrier reducing seepage below percolation flux.

4.3.1.7.4 Rainier Mesa

Rainier Mesa, located approximately 30 km northeast of Yucca Mountain, is underlain by a sequence of welded and nonwelded tuffs similar to those that underlie Yucca Mountain. Precipitation is about double the mean at Yucca Mountain, and percolation is estimated to be about eight percent of precipitation (Wang et al. 1993 [DIRS 108839], p. 676). Tunnels excavated on the Nevada Test Site at Rainier Mesa were generally located in zeolitic tuffs, which are believed to be near full saturation. Faults and joints are abundant in these zeolitic-bedded tuffs. When intersected by tunnels, some of these joints (and especially through-going faults) have yielded significant amounts of water. The seeping features are thought to be pathways for flow from a perched water zone above the zeolitic horizon. Seepage water is geochemically similar to meteoric water and is associated with fast flow paths. Seepage at Rainier Mesa occurs only in tunnels constructed in the zeolites; no seepage has been observed in the tunnel intersecting vitric tuff units. These observations suggest that seepage into tunnels may be localized and restricted to certain flow paths and units. This corroborates the modeling results, which indicate that the seepage fractions are less than one (i.e., that not all waste packages are expected to encounter seepage). More details can be found in *Natural Analogs for the Unsaturated Zone* (CRWMS M&O 2000 [DIRS 141407], Section 6.5.1.2) and Wang et al. (1993 [DIRS 108839], pp. 675 to 681).

4.3.1.7.5 Absence of Seepage into Sealed Exploratory Studies Facility and Enhanced Characterization of the Repository Block Cross Drift Segments

Currently, no natural seepage into the ESF has been observed. Furthermore, no construction water was observed to seep into the ESF main drift as the tunnel boring machine passed the crossover point during the excavation of the ECRB Cross Drift. However, evaporation and moisture removal through ventilation of the ESF are likely to be larger than potential seepage rates, preventing the direct observation of liquid water dripping into the drift.

To study seepage under ambient conditions, sections of the ECRB were sealed by bulkheads in an attempt to reduce unwanted ventilation effects. Two bulkheads were installed in June 1999. During a first entry into the closed-off drift sections in January 2000, moisture was found on the vent line, cables, and pipes. The observed moisture was speculated to be condensate induced by heat sources, such as the tunnel lighting and the tunnel boring machine at the end of the tunnel. A third bulkhead was installed to reduce heat flow from the tunnel boring machine. Drip detection sheets, wind speed sensors, and surface thermocouples were installed. The lights were turned off in July 2000, and the ECRB sections behind the bulkheads were again sealed. The bulkheads were re-opened in January 2001. While parts of the drift were dry, the canvas sheets showed drip marks or were wet, especially in the zone near the Solitario Canyon fault, where there is no overlying PTn. Preliminary evaluations of the drip detection sheets, the chemistry of water samples taken from buckets, and the wind and temperature data suggest that the observed moisture conditions are likely a result of condensation. Although seepage has not been detected, its presence would be consistent with the predictions of the seepage model for the high percolation region near the Solitario Canyon fault.

4.3.1.8 Summary of Uncertainties and Their Treatment

The uncertainty of the parameters estimated with the seepage calibration model (CRWMS M&O 2001 [DIRS 153045]) were considered acceptable given the intended purpose of the model and the use of its results by the seepage model for performance assessment and the seepage abstraction.

Further evaluation of the following sources of uncertainty would reduce the prediction uncertainty of the seepage studies if further reduction were required by users of the seepage model results:

- Uncertainties in the liquid-release test data, specifically those caused by unquantified evaporation losses, should be evaluated. Current and proposed studies (e.g., laboratory, field, theoretical, numerical) may address this issue.

- Because seepage experiments were performed at only a few sites, specific conditions prevailing at other locations and medium- and large-scale spatial variability in hydrogeologic properties may increase the range of potential seepage behavior. Current and planned seepage experiments at additional sites may address this issue.

- For predictions of future seepage into emplacement drifts, extrapolations beyond the conditions encountered during model development, calibration, and validation are performed, which inherently increases the potential for systematic errors. These conceptual uncertainties are addressed through analogue studies, which establish multiple lines of evidence (see Section 4.3.1.7), and through conservative approaches to modeling in the seepage abstraction and TSPA calculations.

Table 4.3.1-2 summarizes the key conceptual and parametric uncertainties, as well as potential data errors affecting the development of seepage-relevant parameters through calibration of a process model against data from liquid-release tests. It should be noted that each conceptual decision, data point, and parameter value remains uncertain, and thus affects the goals outlined in Section 4.3.1.2 to a certain degree. The results of downstream models (specifically the TSPA calculations), as well as the findings of decision and policymakers, will determine whether the remaining uncertainty can be considered acceptable or not.

4.3.1.9 Summary and Conclusions

Seepage into emplacement drifts is considered a key factor affecting the performance of a potential repository at Yucca Mountain. Theoretical analyses, numerical modeling studies, field testing, and observations at analogue sites suggest that seepage into underground openings excavated in unsaturated geologic formations is smaller than the local percolation flux. This is mainly a result of capillary pressure holding water in the formation, diverting it around the excavated opening, and preventing it from entering the drift. The effectiveness of this capillary barrier depends on percolation flux, hydrogeologic properties, and the geometry of the drift.

A sequence of models was used to predict the fraction of waste packages affected by seepage, seepage threshold, and seep flow rates. Seepage process models were calibrated against seepage-relevant data from liquid-release tests. Seepage rates were then calculated over a wide range of parameter values and compiled in an abstraction process. Finally, probability distributions of the key parameters were introduced and conservative approaches were used to arrive at probabilities for seepage into emplacement drifts.

These analyses indicate that seepage fluxes are lower than percolation fluxes, even under conservative modeling, and that only a fraction of the waste packages will encounter seepage.

Naturally, seepage predictions remain uncertain. Some of the identified uncertainties can be further reduced through additional testing and modeling studies.

The overall approach of estimating drift seepage by developing a physically based process model and calibrating it against data from liquid-release tests to obtain site-specific, model-related, and seepage-relevant parameters on the scale of interest was documented in *Seepage Calibration Model and Seepage Testing Data* (CRWMS M&O 2000 [DIRS 119412]). The conceptual model and estimated parameters were then used to develop a database for the subsequent seepage abstraction, as documented in *Seepage Model for PA Including Drift Collapse* (CRWMS M&O 2000 [DIRS 122894]) and *Abstraction of Drift Seepage* (CRWMS M&O 2000 [DIRS 142004]). The abstracted probability functions for seepage rate and seepage fraction supported the TSPA-SR (CRWMS M&O 2000 [DIRS 153246], Section 3.2.4). Additional seepage tests were conducted, providing estimates of reduced uncertainty for both the Tptpmn and Tptpll units. These new results, which are not reflected in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]), confirmed the previous findings and will help reduce prediction uncertainties in future TSPA calculations.

4.3.2 Flow Focusing and Discrete Flow Paths in the Topopah Spring Welded Hydrogeologic Units

4.3.2.1 Introduction

Water percolating downward in the UZ may be focused into discrete flow paths along high-mobility channels. This process tends to concentrate flow, potentially increasing seepage in certain locations, but at the same time reduces the number of waste packages encountering seepage. This section summarizes the modeling studies performed to investigate flow focusing and the characteristics of discrete flow paths that may develop within the UZ fracture network in the TSw. It describes new work that has been conducted since the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]), in the form of sensitivity studies and a scoping analysis, to further assess flow focusing and discrete flow patterns.

Flow focusing and the development of flow channels cannot be directly observed in the field. Therefore, flow-focusing phenomena are mainly addressed through indirect field evidence and the use of models based on physical processes. Related uncertainties stem from uncertainties and ambiguities in conceptual models, characterization data used in these models, and interpretations of modeling results. Unquantified conceptual uncertainties are assessed through analogue studies and other corroborating observations.

Analyses and models supporting the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) used a coarse site-scale grid (100 m or more in horizontal directions) and layer-averaged fracture properties, ignoring the variability in fracture permeability fields within a geologic layer. Detailed flow patterns on a smaller scale, such as fracture spacing, cannot be derived from such a model; therefore, smaller-scale models, such as the drift seepage model, use a higher resolution. This means a gap exists between the site-scale and drift-scale models in modeling flow focusing phenomena. During the seepage abstraction that supported TSPA-SR, flow focusing factors were sampled from probability density functions, which were derived using simplified methods from the weeps model and active fracture model (AFM) (CRWMS M&O 2000 [DIRS 142004], Section 6.4). This approach yielded flow focusing up to a factor of 47 (CRWMS M&O 2000 [DIRS 142004], Section 6.4). This section describes an intermediate-scale model that bridges that gap specifically to address the issue of spatial flow focusing. The effects of faults on flow focusing are not included because of the scale used in the modeling studies.

To quantify flow focusing and address the uncertainty associated with the estimation of flow focusing factors, a stochastic fracture continuum model was developed that honors fracture data from welded tuffs by using measured fracture permeability data. This model was used to study flux allocation mechanisms and flow patterns. It was also used to assess the frequency and flux distributions of major water-bearing flow paths and transport pathways from the bottom of the PTn to the potential repository horizon.

The flow focusing factor (the ratio of local flux to average percolation flux) evaluated in this section is used to determine the upper (spatially variable) boundary flux of the drift-scale model by sampling from the frequency distribution of the flow focusing factor. The modeling results in this section indicate that the flow focusing factors currently used in the TSPA models are very conservative.

4.3.2.2 Goal of the Heterogeneous Flow Model for Site-Scale Domains

Flow focusing along preferential paths, such as well-connected fracture networks, may control patterns of percolation through the highly fractured TSw and directly affect seepage into emplacement drifts. The detailed mechanisms that control unsaturated flow and transport in fractured rocks are site-specific and difficult to characterize. Accurate description of flow focusing processes in unsaturated fractures may be important for the detailed prediction of flow patterns or water seepage into the potential emplacement drifts. However, knowing uncertainty ranges and the average behavior of flow focusing and discrete paths may be more important to the TSPA calculations. This section addresses uncertainties from earlier studies that did not provide sufficient detail on fracture flow at the necessary scale. In addition, drift-scale modeling studies on seepage into drifts show that the amount of water that bypasses or breaks through a capillary barrier of a drift wall depends not only on the capillarity and permeability of the surrounding fracture system, but also on the heterogeneity of the water flux and flow paths (CRWMS M&O 2001 [DIRS 153045], Section 6.1.5).

Various conceptual models have been proposed for describing water flow through the thick, fractured UZ at Yucca Mountain. These models range from continuous flow through a well-connected fracture network (e.g., CRWMS M&O 2000 [DIRS 122797]) to sparse, discrete flow through a small fraction of the fracture network (Pruess et al. 1999 [DIRS 117112]). Modeling approaches used to characterize fracture flow include:

- Continuum modeling (e.g., the effective continuum model) and dual-permeability modeling (Wu et al. 1999 [DIRS 117161]).

- Stochastic modeling representing discrete fractures as currently applied to drift-scale processes (Finsterle 2000 [DIRS 151875]).

The objective of this modeling effort is to understand flow focusing mechanisms and quantify the sensitivity of flow focusing to permeability distributions, correlation structures, and boundary conditions over site-scale domains for the TSw units, from the base of the PTn to the potential repository horizon.

4.3.2.3 Discussion of Initial Results

Initial analyses of flow patterns were conducted for several reports in support of the TSPA-SR: *UZ Flow Models and Submodels* (CRWMS M&O 2000 [DIRS 122797]), *Seepage Calibration Model and Seepage Testing Data* (CRWMS M&O 2000 [DIRS 119412], and *Seepage Model for PA Including Drift Collapse* (CRWMS M&O 2000 [DIRS 122894]. The baseline three-dimensional site-scale model was based on the geologic framework model; it consists of alternating layers of welded and nonwelded tuff units. Hydrologic properties were modeled as uniform within each layer. Fault displacements within the model domain were explicitly taken into account. The hydrologic parameters of the layers were determined by calibrations against all known data, including borehole data regarding saturation and water potentials, temperature profiles, perched water and geochemical information, pneumatic pressure signals, and laboratory core data collected in vertical boreholes and horizontal tunnels.

In *Abstraction of Drift Seepage* (CRWMS M&O 2001 [DIRS 154291], Section 6.4.3), the flow focusing factor was estimated using the AFM. The flow focusing factor was used to conservatively estimate the local enhancement of percolation flux applied to the upper boundary of the drift-scale seepage models. In the drift-scale models, the model domains were populated with stochastically generated permeability values. These fields were conditioned on air-permeability data collected in many boreholes drilled above the crown of the niche excavations in the Tptpmn and Tptpll units. The seepage calibration model was then calibrated against available seepage test results for these units. Previous TSPA-SR estimates of the flow focusing factor were based on interpretations of an AFM parameter (CRWMS M&O 2000 [DIRS 153246]). This parameter did not take into consideration the spatial variability of fracture permeabilities within the welded tuff units, and it was chosen to be conservative (using a flow focusing factor of 50 times the local percolation flux). Details about the drift-scale seepage modeling effort are provided in Section 4.3.1.

4.3.2.4 Flow Focusing Study Developments Since the Initial Results

The three-dimensional flow model in *UZ Flow Models and Submodels* (CRWMS M&O 2000 [DIRS 122797]) used a relatively coarse grid that was unable to resolve potential flow focusing on smaller scales representative of the observed fracture spacings. As a result, the TSPA-SR used the conservative flow focusing factor (CRWMS M&O 2000 [DIRS 153246], Section 3.2.4).

The current effort uses a two-dimensional modeling approach for which a finer grid has been developed. This approach attempts to address uncertainties associated with percolation patterns on the scale of fracture spacing. Fracture permeabilities are assigned to the gridblocks based on the mean value, the standard deviation, and the correlation length of the measured permeability distributions. Using gridblock sizes smaller than fracture spacings and a correlation length longer than the gridblock size results in zones of high permeability channels, representing the behavior of discrete fractures and allowing flow to be focused.

The two-dimensional vertical cross section that forms the basis for the modeling studies summarized in this section has an upper boundary at the bottom of the PTn and a lower boundary at the potential repository horizon. The cross section is 100 m wide and 150 m high. The horizontal dimension of the model is considered sufficient because the correlation length for variability in fracture permeability and spacing is on the order of 1 m. The 150-m vertical extent of the model corresponds to the average distance from the top of the TSw to the top of the potential repository horizon over the potential repository area (CRWMS M&O 2000 [DIRS 114277], Attachment II). The top of the TSw (i.e., the bottom of the PTn) is selected as the upper boundary because the PTn behaves as a porous medium with limited fracture flow, resulting in a more uniform percolation flux (CRWMS M&O 2000 [DIRS 144426], p. 28). Uniform percolation flux (5 mm/yr) boundary conditions are prescribed at this upper boundary as the base case, while nonuniform, spatially distributed percolation flux is used for the supporting sensitivity analyses (see Section 4.3.2.5.2). The two side boundaries are treated as no-flow boundaries; the bottom boundary allows gravitational drainage out of the model.

Only the fracture continuum was modeled in this study because prior modeling studies have shown that at high infiltration rates, the rock matrix in the highly fractured TSw units carries little water under steady-state conditions (CRWMS M&O 2000 [DIRS 122797], Tables 6-22, 6-23, and 6-24). Moreover, modeling indicates that the matrix is not expected to have a major impact on the development of preferential flow paths (i.e., weeps) within the model boundaries because matrix permeability is orders of magnitude lower than the permeability of the fracture network (CRWMS M&O 2000 [DIRS 144426], Table 13). The properties of the fracture system are based on those reported in the *Calibrated Properties Model* (CRWMS M&O 2000 [DIRS 144426], Section 6). There are five different hydrogeologic layers (tsw31 through tsw35) within the two-dimensional model, each of which is represented by different fracture properties (e.g., porosity, fracture spacing, capillary pressure, relative permeability functions).

Fracture permeability is prescribed stochastically, based on measured air-permeability data (Bodvarsson 2001 [DIRS 154669], Attachment 6, pp. 24 to 25). The empirical log-permeability data are represented using a spherical semivariogram model (Deutsch and Journel 1992 [DIRS 100567], p. 23). Details of the methodology for generating stochastic fracture permeabilities are discussed in *Seepage Calibration Model and Seepage Testing Data* (CRWMS M&O 2001 [DIRS 153045], Section 6.3.2 and 6.4.2), which concludes that the fracture permeability near the potential repository is essentially random, with no significant spatial correlation.

Fracture permeability distributions are generated by multiplying the mean fracture permeability of each hydrogeologic unit (CRWMS M&O 2000 [DIRS 144426], Section 6.1.2) by randomly generated multipliers. The software code SISIM (Version 1.203) is used to generate the two-dimensional, spatially correlated permeability field multipliers for each gridblock ($0.25 \text{ m} \times 0.5 \text{ m}$), using a sequential indicator simulation (Deutsch and Journel 1992 [DIRS 100567], p. 151). Two correlation lengths of 1 m (for the base case, Realization #1) and 3 m (for the sensitivity analysis described in Section 4.3.2.5.2) are used to represent weak spatial correlations. The mean and standard deviations of the random permeability field are based on measured air-permeability data (Bodvarsson 2001 [DIRS 154669], Attachment 6, pp. 24 to 25). The fracture permeability, which was generated from field measurements, varies nearly three orders of magnitude, from below 100 millidarcy to over 100 darcy. The upper hydrogeologic units (tsw31, tsw32, and tsw33) have relatively high permeabilities, while the layer immediately above the potential repository horizon (tsw34) has a lower permeability. All fracture properties other than permeability are modeled as constant over each hydrogeologic unit within the entire model domain.

4.3.2.5 Model Results and Analyses

This section summarizes modeling results obtained and analyses conducted since the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]), including base case results, sensitivity analyses, and tracer transport simulations.

4.3.2.5.1 Base Case Results

Figure 4.3.2-1 shows the distribution of simulated liquid mass flux within the two-dimensional model domain using the base case scenario. The figure clearly shows that a number of nearly vertical, high-flux, discrete flow paths develop for this scenario. It also indicates that about five to ten major pathways (or weeps) are present in the upper hydrogeologic layer (above the elevation of -110 m). More pathways are present in the lower layer.

Figure 4.3.2-2 shows the vertical liquid flux at two different elevations: (a) 25 m below the top of the model, and (b) at the bottom of the model (i.e., –150 m). At both elevations, the figure shows a significant spatial variability in the flux, with values ranging from about 0 to almost 30 mm/yr. Statistically, little difference exists between the flow patterns in Figures 4.3.2-2a and 4.3.2-2b, suggesting that flow path characteristics develop within tens of meters from the top of the model and remain statistically similar over the remaining vertical extent of the model (i.e., 100 m). This similarity is illustrated in Figure 4.3.2-3, where the normalized flux (with respect to the mean infiltration rate at the top) is given on the horizontal axis and the flux frequency distribution on the vertical axis. The frequencies are generated by grouping the vertical flux results along an elevation, counting the total found in each group, and calculating the percent contribution relative to the total horizontal distance (or area) in each category. Frequency distributions at four depths are compared: 25, 50, 100, and 150 m. The figure shows similar flux frequency distributions at each elevation, with flow focusing increasing downward.

With percolation normalized to average infiltration, as shown in Figure 4.3.2-3, the flux frequency and distribution at all elevations are statistically similar. The majority of normalized fluxes range from zero to two, with infrequent weeps at high fluxes. The maximum flux that occurs in the system is generally about five to six times more than the prescribed infiltration rates at the upper boundary. This flow focusing factor is considerably lower than what is currently used in the TSPA-SR models, in which local fluxes were increased by up to a factor of 47 over prevailing percolation flux (CRWMS M&O 2000 [DIRS 142004], Section 6.4.3.2). The wide spread of flow focusing factors used in TSPA-SR yields a wider, albeit conservative, distribution of drift seepage.

4.3.2.5.2 Sensitivity Studies in Support of the Main Conclusion

Several sensitivity analyses were performed; the scenarios described in the following text are summarized in Table 4.3.2-1. These sensitivity studies used:

- Different infiltration rates
- A second realization for fracture permeability (Realization #2)
- A different correlation length of 3 m to generate the permeability (Realization #3)
- Different infiltration patterns (uniform versus pulse).

Figure 4.3.2-4 shows that the flux frequency and distribution for all the infiltration rates (with infiltration rates on the top boundary varying from 1 to 500 mm/yr) in terms of normalized percolation flux are statistically similar. This indicates that discrete flow paths are insensitive to net infiltration rates.

The second realization of fracture permeability (Realization #2) (Bodvarsson 2001 [DIRS 154669], Attachment 14, pp. 25 to 32) is created by initiating the random number generator with a different seed number (Deutsch and Journel 1992 [DIRS 100567]). This realization yields a percolation distribution statistically similar to the first realization. Simulations performed using the 3-m correlation length for the permeability field (Realization #3) result in fewer but slightly larger weeps. The distribution pattern for this realization is similar to the pattern shown in Figure 4.3.2-3 for the 1-m correlation length case. The sensitivity study with the nonuniform infiltration boundary condition (Realization #4) shows that if a spatially variable infiltration is used, the flow patterns behave as if the flux condition at the upper boundary were uniform.

As discussed above, frequency plots for all the sensitivity studies are similar, suggesting that a general frequency plot for the flow-focusing factor can be developed for use in TSPA abstraction. The conclusions of these sensitivity studies support those of the base case. The flow focusing factor is likely to be considerably lower than what is currently used in the TSPA-SR models (CRWMS M&O 2000 [DIRS 153246], Section 3.2.4.3).

4.3.2.5.3 Results with Tracer Transport

Tracer transport analyses are used with the two-dimensional model to provide additional insight into flow focusing and discrete pathways. The results of some of the transport modeling using the base case flow model are presented in this section (i.e., uniform top infiltration flux and 1 m correlation length for fracture permeability). A conservative, nonsorbing tracer with a molecular diffusion coefficient of $D_m = 3.2 \times 10^{-11}$ m^2/s at constant concentration is prescribed at the top model boundary. Under steady-state flow, the tracer is transported into the model domain from the top by advection and diffusion. Figure 4.3.2-5 shows the concentration contours in the model domain after one year of tracer release at the top boundary. Note that all matrix blocks are omitted in these simulations, so retardation (caused by matrix diffusion and sorption) is implicitly neglected. The results show areas of high tracer concentrations (Figure 4.3.2-5), indicating the existence of nonuniform, complex transport pathways (i.e., the development of several fast-flow channels, or fingering). A comparison of Figures 4.3.2-1 and 4.3.2-5 indicates that faster transport pathways generally follow faster flow pathways. Therefore, concentration distributions within the model domain serve as indicators of preferential flow.

4.3.2.6 Abstraction for Total System Performance Assessment

As Figure 4.3.2-4 demonstrates, the results of the analyses can be used to estimate the flow focusing factor for the seepage abstraction. The normalized flux distributions are similar, and it is reasonable to define a single distribution that applies to all expected percolation rates. A regression curve with confidence bands, summarizing the results of all the simulations, is shown in Figure 4.3.2-6.

The distribution shown in Figure 4.3.2-6 cannot be used directly to define the flow focusing factor for seepage abstraction because the factor is defined in such a way that it is always greater than 1. The part of the normalized flux distribution that is below 1 is accounted for implicitly in the abstraction model (CRWMS M&O 2001 [DIRS 154291], Section 6.4.3.2). However, two important observations must be made: (1) the flow enhancement indicated by these simulations is usually less than three and always less than about six, and (2) there is little spread in the results from different simulations.

In contrast, the uncertainty distributions for the flow focusing factors defined for the TSPA-SR seepage abstraction (CRWMS M&O 2000 [DIRS 153246]) were quite broad, ranging as high as 47 (CRWMS M&O 2001 [DIRS 154291], Section 6.4.3.2). The distributions were derived using a method developed to estimate the spacing of actively flowing fractures on scales below the resolution of the UZ site-scale model. In fact, two methods were used to estimate the flowing-fracture spacing; one implied relatively small spacings averaging 1 to 2 m, while the other implied larger spacings averaging 20 to 30 m (CRWMS M&O 2001 [DIRS 154291], Table 15). The lower values (from the unsaturated active fractures method) are more consistent with the results presented here. For the seepage abstraction, an uncertainty distribution was defined that spanned both methods. The inclusion of the larger focusing factors was considered to be conservative, and it has been shown that larger flow focusing factors tend to produce higher radionuclide doses because of increased total seepage (CRWMS M&O 2000 [DIRS 153246], Section 5.2.1.2).

The average flow enhancement in the results shown in Figures 4.3.2-4 and 4.3.2-6, considering only the part of the normalized-flux distribution above 1, is slightly less than a factor of 2. These results are bounded by an exponential distribution with a mean of 2 (truncated at 1). Thus, the results indicate that it would be more realistic to use a flow focusing factor of about 2 in TSPA simulations, rather than the distributions of focusing flux that were defined for the seepage abstraction.

The results presented here are used to define the flow focusing factor for the TSPA sensitivity analyses presented in Volume 2 (McNeish 2001 [DIRS 155023], Sections 3.2.2.3, 3.2.2.7, and 4). The distributions shown in Figures 4.3.2-4 and 4.3.2-6 represent spatial variability in the amount of flow focusing. However, the current seepage abstraction does not allow for spatial variability of the flow focusing factor (CRWMS M&O 2000 [DIRS 148384], Section 6.3.1.2), and there may be additional sources of uncertainty that have not been addressed in these analyses. It is preferable to use an uncertainty distribution set to the bounding exponential distribution with a mean of 2. This adjustment would acknowledge that uncertainty exists in the amount of flow focusing, rather than using a single deterministic value of approximately 2 for the sensitivity analysis. In this way, the higher flow focusing factors would be accounted for in at least some of the TSPA realizations.

4.3.2.7 Multiple Lines of Evidence

Evidence of flow focusing occurring at Yucca Mountain can be inferred from observations of calcite and opal occurring in some cavities in the Yucca Mountain UZ. These secondary minerals formed as deposits precipitated by percolating water (Paces et al. 2000 [DIRS 154412]). The mineralization indicates that seeps are not regularly spaced in the underground excavations and that not all fractures sustain flow. Furthermore, many cavities represent sites of seepage that have remained stable for millions of years (Marshall et al. 2000 [DIRS 151018]).

In the excavation of Niche 1 in the vicinity of the Sundance fault, a damp feature was observed (DOE 2001 [DIRS 153849], Figure 4-18). The Sundance fault is one of several faults and features with bomb-pulse signals detected from chlorine-36 measurements (Fabryka-Martin et al. 1997 [DIRS 100145]). The feature was nearly vertical, and it was approximately 0.3 m wide and 3 m long. It dried out before a bulkhead could be installed to prevent contact with ventilation air and has not fully rewetted after two years of observation with the bulkhead closed.

Another damp feature was observed during the excavation of ESF Niche 1 (Station 35+66), the first niche excavated for the seepage studies. This feature, at the end of the niche, was wet to the touch and had a darker color until ventilation dried it up (Wang et al. 1999 [DIRS 106146]).

Nearly uniform distributions of water potential in the Topopah Springs welded tuff (Rousseau et al. 1997 [DIRS 100178], p. 45, 1999 [DIRS 102097], p. 123) and areally near-uniform perched water chloride concentrations indicate that the effective flow focusing factor is small, or generally less than two. This indicates that there are many small flow paths instead of a few large ones, and that the small flow paths are separated by large regions with reduced percolation.

4.3.2.8 Summary of Remaining Uncertainties

Uncertainties associated with the flow focusing studies have been discussed in the preceding text. The main uncertainties associated with these studies can be summarized as: (1) accuracy in describing the fracture permeability fields in the units between the PTn and the potential repository, (2) use of a fracture continuum model, and (3) the effects of matrix heterogeneity. A more complete list of the uncertainty issues particular to flow focusing and their treatment is given in Table 4.3.2-2.

4.3.2.9 Summary and Conclusions

Modeling studies using a stochastic fracture continuum model have been conducted to evaluate flow focusing through fractures from the bottom of the PTn to the potential repository horizon. These studies were carried out using a 100-m wide and 150-m deep two-dimensional cross section covering the upper five TSw hydrogeological units at Yucca Mountain. Mean fracture parameters used in the simulations were obtained from the *Calibrated Properties Model* (CRWMS M&O 2000 [DIRS 144426], Section 6). Heterogeneous fracture permeability distributions were generated using a stochastic approach conditioned on field-measured air-permeability data. The studies considered various percolation fluxes, correlation lengths, and uniform and nonuniform percolation-flux boundary conditions. The results provide a quantitative analysis of flow focusing. All simulation results indicate that the flow focusing factor is likely to be much smaller than the value used in previous TSPA calculations; therefore, the TSPA calculations are conservative with respect to flow focusing issues, since they use a flow focusing factor that may be an order of magnitude higher than that suggested by the scoping studies presented in this section. This means that the current conservative TSPA approach may overestimate the seepage flux. In addition, the sensitivity analyses indicate that frequency distributions of normalized flux are insensitive to the magnitudes or spatial distributions of percolation fluxes specified on the upper boundary. The frequency distributions are also insensitive to the spatial correlation structure of the permeability fields within the UZ. The flux frequency distribution function may be incorporated into the TSPA for a more realistic representation of the UZ flow and transport field.

4.3.3 The Effect of Rock Bolts on Seepage

This section summarizes the modeling and uncertainty studies performed to evaluate the potential for rock bolts to enhance seepage above that predicted by the models summarized in Section 4.3.1. Model results abstracted for the TSPA-SR (CRWMS M&O 2000 [DIRS 153246], Section 3.2.4) suggested that the presence of rock bolts would enhance seepage; however, more detailed models, recently developed and summarized here, show that rock bolts do not enhance seepage.

4.3.3.1 Introduction

The use of grouted rock bolts is one proposed method of providing ground support for emplacement drifts. Grouted rock bolts might be used in the Tptpmn, but not in the Tptpll, the other rock unit in which emplacement drifts would be located. Rock bolts are steel rods grouted into a borehole normal (i.e., perpendicular) to the drift wall. They accomplish two purposes: they bind the mass of rock above the drift to prevent large rockfalls, and they provide an anchor point for the steel mesh that is placed against the drift wall to prevent raveling (i.e., small rockfalls). Rock bolts present a concern with respect to seepage because they may provide a direct flow conduit to the drift wall. If so, they increase the likelihood that a flowing fracture will be intersected and flow will be diverted to the drift wall to become seepage.

Uncertainties specific to modeling the effect of rock bolts on seepage (in addition to the general uncertainties for seepage models; see Section 4.3.1) are summarized below.

Properties of the Grout Material–How the properties of the grout material, modeled as the conduit for flow diversion toward the drift wall, will change over time is unknown. Because seepage is a process relevant to long-term performance, knowledge of the changing properties as the grout degrades over time are necessary to evaluate the effects of rock bolts on seepage. This uncertainty is addressed by evaluating seepage enhancement over a large range of grout properties. The steel rod portion of the rock bolt system is modeled as impermeable or completely absent. Any contribution to seepage enhancement due to corrosion of the steel rod, either at the steel-grout interface or within the rod itself, is adequately addressed by varying the properties of the grout surrounding the rod.

Properties of the Formation Surrounding the Rock Bolt–The properties of the formation surrounding the rock bolt are heterogeneous on scales larger than the rock bolt, as evidenced by the distinct permeabilities measured at ESF Niche 3 (located at Station 31+07), Niche 2 (Station 36+50), and Niche 4 (Station 47+88) (CRWMS M&O 2001 [DIRS 153045], Section 6.2.2), and they are uncertain because evaporation is considered to have a negligible effect in the testing and calibration process (CRWMS M&O 2001 [DIRS 153045], Section 5.6). This uncertainty is addressed by evaluating seepage enhancement for several values of the formation capillary strength parameter, $1/\alpha$, which is potentially the most uncertain parameter.

Use of a Homogeneous Model–The use of a homogeneous model, which neglects the heterogeneities on scales smaller than the rock bolt, may affect the results. This uncertainty is addressed by comparing base case seepage results from this model to those from a heterogeneous model.

4.3.3.2 Goal of the Rock Bolt Model

The goal of the rock bolt model is to evaluate the potential for rock bolts to enhance seepage above the levels predicted by the base case seepage model (Section 4.3.1). The rock bolt model is presented in *Seepage Model for PA Including Drift Collapse* (CRWMS M&O 2000 [DIRS 153314], Section 6.7) and *Abstraction of Drift Seepage* (CRWMS M&O 2001 [DIRS 154291], Section 6.4.1).

4.3.3.3 Discussion of Initial Results

In the initial version of *Seepage Model for PA Including Drift Collapse* (CRWMS M&O 2000 [DIRS 122894], Section 6.7), the treatment of rock bolts as a seepage-enhancing factor considered an extremely simple model for rock bolts. Rock bolts were modeled as "needles" extending from the drift wall (the last grid node before the drift wall) vertically downward into the drift, unlike bolt holes, which extend upward away from the drift. Because the "needle" is a single connection, there is no opportunity for lateral flow away from it near the drift wall. The size and properties of this node were unmodified with respect to the surrounding grid. This is in contrast to an actual rock bolt hole, which would have a smaller horizontal cross section and, depending on the properties of the material in the hole (or lack thereof), might create a permeability or capillary barrier and divert flow. These simplifications are likely to significantly impact the results. Seepage enhancement was found to stabilize for needle lengths of 0.15 to 0.25 m. The seepage enhancement for one needle was found to be 3 percent.

4.3.3.4 Discussion of Updated Results

No new analysis or model of the effect of rock bolts on seepage was presented in the update to *Seepage Model for PA Including Drift Collapse* (CRWMS M&O 2000 [DIRS 153314], Section 6.7).

4.3.3.5 Discussion of Current Results

A more complete model of the effect of rock bolts, presented in this section, considers several factors, including:

- The properties of degraded grout and rock bolt material, including the case in which the rock bolt and grout are completely removed from the hole such that the rock bolt hole is a capillary barrier
- The dimensions of the rock bolt and grout
- Uncertainty in the hydraulic properties of the formation
- A range of percolation rates
- The possibility for lateral diversion away from the rock bolt at or near the drift wall
- Rock-bolt density and orientation.

A sketch of the conceptual model for how a rock bolt hole and percolation may interact to enhance seepage (Figure 4.3.3-1) shows that flow along a fracture may encounter a rock bolt hole and either be diverted around the hole or enter the hole. How much flow enters the hole and how much is diverted around it depends on the dimensions of the hole, the angle of the fracture with respect to the hole, the rate of flow, the channeling of flow in the fracture, the hydraulic properties of the grout filling the hole (or the absence of grout, if it has completely degraded), and the local saturation of the grout. Flow that enters the hole will not necessarily result in seepage. The head (or reduction in capillary pressure) at the collar of the hole (i.e., where the hole intersects the drift wall) may not be sufficient to induce seepage, especially if there are pathways for the water to flow back into the formation and be diverted around the drift. Similarly, if seepage is already occurring without the presence of rock bolts, enough diversion capacity may exist such that the rock bolts will not increase seepage.

The proposed use of ground support is documented in *Ground Control for Emplacement Drifts for SR* (CRWMS M&O 2000 [DIRS 146022], Section 6.2). The proposed rock bolt and grout dimensions are 3 m long (CRWMS M&O 2000 [DIRS 146022], Section 6.5.2.2), with a rock bolt diameter of 0.0254 m and a grout annulus thickness of 0.00635 m (CRWMS M&O 2000 [DIRS 146022], Table 4-10). The rock bolts would be emplaced with a lateral spacing of 1.5 m (CRWMS M&O 2000 [DIRS 146022], Section 6.5.2.2). The properties and expected longevity of the rock bolt and grout system are documented in *Longevity of Emplacement Drift Ground Support Materials* (CRWMS M&O 2000 [DIRS 150202], Section 6.4). The design permeability of newly emplaced grout is less than 10^{-18} m^2 (10^{-12} m/s) (CRWMS M&O 2000 [DIRS 150202], Sections 6.4.1 and 6.4.3.1), and its expected life at that permeability is 300 yrs (CRWMS M&O 2000 [DIRS 150202], Section 6.4.3.1).

A refined model that includes a range of properties for the grout and the formation and a range of percolation rates has been prepared. The model uses a two-dimensional, radially symmetric grid with a vertical symmetry axis generated using the software iTOUGH2 V4.0. The grid size is

0.1 m, with finer discretization (down to 0.001 m) at the interface between the grout and the surrounding rock. Because this is a radially symmetric grid, the drift opening, which is created using the software routines MoveMesh V1.0 and CutNiche V1.3, is spherical instead of cylindrical. Knight et al. (1989 [DIRS 154293], p. 37) find that seepage exclusion from a cylindrical cavity is similar to that from a spherical cavity of twice the radius. This is explained by relating the seepage exclusion potential of an opening to the total curvature of the boundary of the opening. The total curvature of a cylindrical cavity can be described by two radii, one finite and one infinite (perpendicular and parallel to the axis of the cylinder, respectively), while that of a spherical cavity can be described by two radii that are equal and finite. In the model, the equivalent radius used for the spherical "drift" is twice that of the design drift radius.

For the base case, seepage into the opening without any rock bolts is modeled. Percolation rates of 5, 14.6, 73.2, 213, and 500 mm/yr are applied uniformly to the upper model boundary, as used in *Seepage Model for PA Including Drift Collapse* (CRWMS M&O 2000 [DIRS 153314], Section 6.3.7). Parameter Set A from that report, as well as the alternative $1/\alpha$ values of 400 and 200 Pa (CRWMS M&O 2000 [DIRS 153314], Section 6.3.5), are used for the excavation-disturbed zone in the Tptpmn rock unit surrounding the drift. A constant zero capillary pressure is specified at the drift wall boundary, a gravity drainage condition at the lower boundary (assigned in the grid using the software routine AddBound v 1.0, and a no-flow condition at the lateral boundary, all of which are consistent with the current models of seepage at Yucca Mountain (CRWMS M&O 2001 [DIRS 153045], Section 6.3.2.4; CRWMS M&O 2000 [DIRS 153314], Section 6.3).

To investigate the impact of a rock bolt on seepage, only the case of a rock bolt hole extending vertically upward from the crown of the drift is modeled. This case is sufficient to investigate the impact of the presence of the rock bolt hole on seepage (see Section 4.3.3.8). Three slightly different grids (Cases 1 to 3) are prepared to explore diversion capacity away from the rock bolt hole. Case 1 allows flow between the rock bolt hole and the surrounding rock along the entire length of the bolt hole. Case 2 restricts flow between the rock bolt hole and the surrounding rock for 0.1 m above the crown of the drift. Case 3 restricts flow between the rock bolt hole and the surrounding rock for 0.5 m above the crown of the drift. Cases 2 and 3 represent scenarios in which the first feature capable of carrying flow away from the rock bolt hole is found 0.1 m or 0.5 m, respectively, into the hole. A 0.0254-m radius bolt hole with a 0.0127-m radius rock bolt and a 0.0127-m grout annular thickness is modeled. These features are added to the grid using the software routine AssignRock V1.0. The difference between the design grout annular thickness and that modeled is conservative. The modeled rock bolt hole has less potential as a capillary barrier to exclude in-flow, a larger surface area to intercept flow, and more potential to conduct flow to the drift wall. Thus, results from this model will overestimate the seepage enhancement due to rock bolts; however, results show that this conservatism is not a concern with respect to accuracy.

Because the greatest impact of the rock bolts on seepage may come many thousands of years into the future (after cooldown and rewetting of the potential repository horizon and during wetter future climates), the grout is not likely to retain its design hydraulic properties. It may even disintegrate completely, leaving an open hole. A range of properties is used for the grout to address this uncertainty. Figure 4.3.3-2 shows the 13 parameter combinations evaluated. The lower-left combination (permeability = 10^{-18} m^2; $1/\alpha = 10^7$ Pa) corresponds to the design grout, while the upper right combination (permeability = 10^{-10} m^2; $1/\alpha = 10$ Pa) corresponds to an open rock bolt hole. The other parameter combinations are selected to be equally spaced between the end points.

To summarize, a sensitivity study was performed in which several model parameters and the grid were varied to adequately address uncertainties in the conceptual model and input parameters. The varied parameters were:

- The permeability and capillarity of the grout
- The capillarity of the formation
- The percolation rate
- The length over which flow is restricted from the rock bolt into the formation adjacent to the drift wall.

Details of the model and sensitivity study are presented in Bodvarsson (2001 [DIRS 154669], Attachment 3, pp. 62, 63, and 68 to 70). The sensitivity study uses the software TOUGH2 V1.5 to simulate unsaturated flow.

No seepage enhancement is predicted for any of the combinations of percolation rate, formation parameter, grout parameter, and numerical grid. This result is different from the previous "needle" calculation, where 3 percent seepage enhancement was shown for one rock bolt. However, the current result is understandable, especially considering two key points about the previous simulation. First, the area onto which flow may be incident, if the lateral surfaces are considered, is 1.25 m^2 in the previous model, as opposed to 0.24 m^2 in the current model (a ratio of 5 to 1). If only the horizontal surfaces are considered, the ratio increases to more than 100 to 1. Second, the parameters from the seepage calibration model, which are used in the seepage model for TSPA (CRWMS M&O 2000 [DIRS 153314]), are predicated on the use of 0.05 m connection distances between the drift wall and the first node adjacent to the drift wall (CRWMS M&O 2001 [DIRS 153045], Sections 1, 6.3.2.2, and 6.4.2.2). The previous calculation found significant seepage enhancement only when that connection was 3 to 5 times the recommended length, restricting the lateral flow away from the rock bolt.

4.3.3.6 Abstraction for Total System Performance Assessment

As discussed above, *Seepage Model for PA Including Drift Collapse* presents a simple estimate of the possible effects of degraded rock bolts on seepage (CRWMS M&O 2000 [DIRS 122894], Section 6.7). Based on that estimate, seep flow rates were conservatively increased by 50 percent to account for the effect of rock bolts and drift degradation in the seepage abstraction for the TSPA-SR (CRWMS M&O 2000 [DIRS 142004], Section 6.3.1). Additional work that had not been included in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]), did not address new models of the effects of rock bolts on seepage (CRWMS M&O 2000 [DIRS 153314], Section 6.7; CRWMS M&O 2001 [DIRS 154291], Section 6.4.1). The more detailed study of rock bolt effects presented here found no significant increase in seepage because of either intact or degraded rock bolts. Thus, it would be appropriate to eliminate the increase in seepage due to rock bolts. A possible revision that includes this change is discussed in Section 4.3.4.6.

4.3.3.7 Multiple Lines of Evidence

Because of the specificity of this investigation (i.e., seepage enhancement resulting from rock bolts), multiple lines of evidence to support the conclusions are rare, if they exist at all. The lack of seepage enhancement due to rock bolts also complicates the use of corroborating evidence. The lack of observations of seepage enhancement due to rock bolts in similar situations is not necessarily proof that seepage cannot be enhanced by rock bolts in similar situations. Though the use of multiple lines of evidence may be complicated by these factors, it may be useful to discuss evidence that contradicts the conclusions reached in this section.

The results of this analysis appear to run counter to observations of occasional dripping at rock bolts in the ESF and associated tunnels. There are several factors associated with these rock bolts that suggest this dripping is not an enhancement of background-percolation seepage. The type of rock bolt used in the ESF and associated tunnels is not the same one that will be used in the emplacement drifts; in the current tunnels, hollow steel bolts are used. These bolts are expanded against the sides of the hole using water pressure (the end of the bolt is capped), possibly leaving water inside the bolt (which may drip out). In addition, temperature, humidity, and pressure variations in the tunnels could lead to condensation inside the hollow bolts that would lead to dripping. This water would not come from the rock formation because the bolt is impermeable. Lastly, water that was used in the mining of these tunnels and for drilling of the rock bolt holes may be condensing and creating saturated conditions on the outside of the bolts because the bolts are better thermal conductors than the surrounding rock.

The analysis results also appear to run counter to observations of seepage enhancement caused by rock bolts in saturated zone tunnels. However, in the saturated zone, the concept of the tunnel as a capillary barrier does not apply. By definition, the potential at all points around the drift is zero, so the seepage percentage is 100 percent. Rock bolts then add to the surface area of the drift or to the likelihood that the drift will intersect a flowing feature, and thus must enhance seepage. As demonstrated above, the ability of the drift to act as a capillary barrier in the UZ is essential to its being able to divert flow away from the rock bolt and around the drift.

4.3.3.8 Summary of Uncertainties and Their Treatment

Table 4.3.3-1 presents a summary of uncertainty issues related to rock bolts. Additional issues may be classified as conceptual uncertainties. These are discussed below, and justifications are given for why they do not impact the model.

1. The use of a homogeneous permeability field in this model may bias it toward lower seepage. This concern is unjustified because comparison of the seepage percentage predicted by this model with that predicted by the seepage model for performance assessment (Figure 4.3.3-3) indicates that, for the formation parameters used, no significant difference exists. There is more difference in the seepage percentage between the different formation parameters than there is between the models. Further, because the result of concern is seepage enhancement rather than seepage percentage,

the use of a consistent model (i.e., a homogeneous one) for both the base case and the rock bolt simulations is the important issue. The impact of homogeneity or heterogeneity on seepage enhancement is considered a second-order effect.

2. The use of a vertical rock bolt rather than an inclined rock bolt minimizes the area onto which percolation is incident. Current simulations show that, for certain grout parameter combinations, flow enters even a vertical rock bolt hole from the sides, enhancing percolation through the grout with respect to the percolation around the hole. The key to the lack of seepage enhancement is the potential for sufficient lateral diversion at or near the drift wall to direct flow in the hole away from the hole. There will be even more diversion potential for an inclined hole because the height of any "disconnected" length of the hole will be less, and the diversion potential along the angled portion of the drift wall is much greater than at the crown of the drift.

Alternative models for the investigation of seepage enhancement because of rock bolts include:

- Continuum models employing multiple realizations of heterogeneous permeability fields
- Discrete fracture models
- Models that include inclined rock bolt holes.

The discussion above suggests that the first and third alternative models are unlikely to give significantly different results. The key element of the discrete fracture model (i.e., discrete features for flow into or out of the bolt hole) is adequately captured by the two current models, in which the bolt hole is disconnected from the formation near the drift wall.

4.3.3.9 Summary and Conclusions

The potential for seepage enhancement into emplacement drifts in the Tptpmn due to rock bolts has been evaluated, and no evidence of seepage enhancement was found. Parameter uncertainties for the grout and the formation are addressed through sensitivity studies using multiple parameter combinations. Grout permeability varied from 10^{-18} to 10^{-10} m^2, and capillarity varied from 10^7 to 10^1 Pa. Tptpmn formation capillarity varied between 200 and 589 Pa. Sensitivity studies were used to address conceptual uncertainties about the appropriate modeling of flow restrictions away from the rock bolt adjacent to the drift wall because of a lack of fractures to conduct flow. Three numerical grids were used: the first has a full-connection between the rock bolt and the formation adjacent to the drift wall, the second restricts flow between the rock bolt and the formation for 0.1 m above the drift wall, and the third restricts flow between the rock bolt and the formation for 0.5 m above the drift wall. A range of percolation rates, from 5 to 500 mm/yr, was used to adequately cover the rates expected at the potential repository horizon.

Evidence of seepage enhancement due to rock bolts in the UZ and the saturated zone was found not to be relevant as evidence against the conclusions reached. Processes that will not be found in the emplacement drifts (e.g., short-term release of mining water, use of hollow rock bolts, saturated conditions surrounding the drift) are concluded to be responsible for the observed seepage enhancement in the ESF and associated tunnels.

The conclusion of this investigation of the potential for enhancement of seepage into emplacement drifts in the Tptpmn caused by intact or degraded rock bolts is that there is no significant enhancement of seepage, and that rock bolts may be neglected as a seepage-enhancement factor for performance assessment.

4.3.4 Drift Degradation

4.3.4.1 Introduction

Analyses and models supporting the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) used a three-dimensional model to examine simple drift degradation scenarios, which are summarized in Section 4.3.4.3. Studies conducted after the TSPA-SR, which are discussed in Section 4.3.4.4, utilize significantly more detailed drift degradation profiles based on a discrete region key-block analysis (CRWMS M&O 2000 [DIRS 151635]; DTN: MO0010RDDAAMRR.002 [DIRS 154048]). By using the discrete region key-block approach, more realistic representations of drift degradation are achieved, resulting in an improved understanding of the impact of heterogeneity on flow fields.

Drifts in which waste packages will be emplaced are subject to degradation in the form of permeability changes in the rock around the drift and rockfall from the drift ceiling. The former results from the excavation process (i.e., the stress release caused by the excavated cavity); the latter results from the multiple fractures present in the rock, which in turn could cause the blocks created by intersecting fracture sets to become loose and fall into the drift. Either type of drift degradation will create uncertainty if seepage estimations are based on a drift without degradation. This uncertainty is addressed by: (1) defining a heterogeneous permeability model at the drift scale that is consistent with field data, (2) selecting the best-calibrated parameters associated with the Tptpmn and the Tptpll lithostratigraphic units in which the potential repository will be situated, (3) considering the possible ways that the drift can degrade, (4) selecting scenarios of degradation, (5) implementing these scenarios as model inputs, and (6) calculating the change in seepage for each of these scenarios.

The effects of drift degradation on potential seepage into drifts at Yucca Mountain as used in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) are documented in *Seepage Model for PA Including Drift Collapse* (CRWMS M&O 2000 [DIRS 122894], Sections 6.3, 6.4, and 6.6.4). The major change to this AMR (CRWMS M&O 2000 [DIRS 153314], Section 6.1) was the modification of the drift boundary condition, as discussed in Section 4.3.4.3. New studies used modified drift degradation scenarios, which are presented in Sections 4.3.4.4 and 4.3.4.5.

4.3.4.2 Goals of Drift Degradation Submodel

The goals of the drift degradation submodel are as follows:

1. To use a heterogeneous model, with the best available calibrated parameters, to study the impact of drift seepage due to heterogeneity of flow fields and degradation effects

2. To identify possible cases for drift seepage and propose scenarios or cases for study

3. To perform simulation studies on these cases and estimate the impact of drift degradation on seepage.

4.3.4.3 Discussions of Revision 00 and Revision 01 Results

In *Seepage Model for PA Including Drift Collapse* (CRWMS M&O 2000 [DIRS 122894], Section 6.6), simulations were performed to calculate seepage values for a range of values of percolation flux at the drift to study the effects from various processes, such as excavation-induced drift degradation, and to provide results as input to the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]).

The results in a revision to *Seepage Model for PA Including Drift Collapse* (CRWMS M&O 2000 [DIRS 153314], Section 6.6) are different. Changes make the revised AMR consistent with the *Seepage Calibration Model and Seepage Testing Data* (CRWMS M&O 2001 [DIRS 153045], Sections 5 and 6). Additionally, the seepage calibration model provided results for the Tptpll lithostratigraphic unit, which were not available at the time the initial report was issued.

A heterogeneous permeability field of the fracture continuum is the basis for the conceptual model used to examine the heterogeneity of flow fields. The numeric representation was generated using parameter sets (described below) in conjunction with the SISIM module of GSLIB V2.0. The three-dimensional block defined by the generated heterogeneous field is 20 m tall, 15 m wide, and 5.23 m along the drift axis. It contains a drift that is 5.5 m in diameter and positioned to have an overlying thickness of 9.75 m, an underlying thickness of 4.75 m, and a distance to either side of 4.75 m. The vertical cross-sectional dimensions of the block were chosen to be wide enough to capture flow diversion around the drift (Philip et al. 1989 [DIRS 105743], p. 21, Figure 1). The heterogeneous field was chosen so that flow focusing or channeling within the scale of the model is accounted for in the simulation.

Flow calculations were performed using the numerical simulator ITOUGH2 V3.2_drift. A number of routines were also used for preprocessing of inputs for this simulator, as listed in Table 1 of *Seepage Model for PA Including Drift Collapse* (CRWMS M&O 2000 [DIRS 153314]).

Three parameter sets for repository placement, obtained by calibration against field data from relevant formations, are used in this study. The first set, Set A ($k_{FC} = 1.38 \times 10^{-12} m^2$; $1/\alpha = 589$ Pa; $n = 2.55$; $\sigma = 1.93$), is the set of calibrated mean parameters for the Tptpmn unit given by the seepage calibration model (CRWMS M&O 2001 [DIRS 153045]; DTN: LB0010SCMREV01.002 [DIRS 153393]). Note that k_{FC} is the calibrated mean permeability, α and n are the van Genuchten parameters, and σ is the standard deviation of $\ln k_{FC}$.

The second parameter set, Set B ($k_{FC} = 1.38 \times 10^{-11} m^2$; $1/\alpha = 871$ Pa; $n = 2.57$; $\sigma = 1.93$), is the set of calibrated mean parameters chosen for the Tptpll unit (DTN: LB0010SCMREV01.002 [DIRS 153393]). Note that $\sigma = 1.93$ is used for both sets as a more conservative value (details are included in *Seepage Model for PA Including Drift Collapse* [CRWMS M&O 2000 (DIRS 153314)], Section 6.3.3).

An additional parameter set, Set B′, is also considered for the Tptpll unit. It is identical to Set B except that it uses a $1/\alpha$ value of 537 Pa. Set B′ is intended to compensate for the effect of lithophysal cavities, which tend to increase seepage (CRWMS M&O 2001 [DIRS 153045], Section 6.3.3.3).

Drift degradation may occur in three ways:

1. Rockfall from the ceiling of the drift
2. Loosening of rock blocks that increases fracture apertures (fracture dilation)
3. Extended rock failure in the drift ceiling.

Based on these possibilities, a drift degradation submodel was designed to evaluate the impact of drift degradation on seepage. The submodel is shown in Figure 4.3.4-1 as four alternative scenarios, discussed in the following paragraphs.

Rockfall from Drift Ceiling–*Drift Degradation Analysis* used the key-block theory to calculate rockfall probability in the drifts under various scenarios, based on fracture maps in the ESF (CRWMS M&O 2000 [DIRS 151554], Tables 20 to 21, 26 to 27, 35 to 36, 41 to 42). Based on the probabilities developed for the Tptpmn unit, the number of key blocks per kilometer of the drift was calculated to be fewer than 44 over these scenarios, and the volume of total rockfall per kilometer to be less than 36 m^3. This implies that rockfall occurs on the average of one block every 23 m and that the mean size of the block is about 0.8 m^3. This is confirmed by the finding that 80 percent of the blocks are smaller than 1 m^3 (CRWMS M&O 2000 [DIRS 151554], Figures 19 to 20, 27 to 28, 32 to 33, 36 to 37). Hart (Brekke et al. 1999 [DIRS 119404], p. E-12) used a two-dimensional discrete-element method and found rockfall to occur at the springline of the drift, with the size of the block depending on the modeled fracture spacing. To study the effect of rockfall on seepage, two calculations were made, one in which a 1.0 m^3 block was taken out from the crown of the drift and one in which the 1.0 m^3 block was taken out at the springline (Figure 4.3.4-1, top right and left).

Fracture Dilation–Stress is relieved at the drift because of excavation, and fractures are expected to dilate at certain areas around the drift (Figure 4.3.4-1, lower left). Such fracture dilation depends on the orientation of the fracture set and generally occurs within one drift radius (Brekke et al. 1999 [DIRS 119404], Figures E-5, E-11, and E-13). An increase in fracture aperture generally causes an increase in fracture permeability and a decrease in $1/\alpha$ value. The measured increase in permeability from the pre-excavation to the post-excavation values (Wang et al. 1999 [DIRS 106146], p. 328; DTN: LB0011AIRKTEST.001 [DIRS 153155]) is a result of this effect. Both Set A and Set B, which are based on in situ post-excavation calibration results, already have taken this increase into account. This means that the rock properties used already represent the total effect of the near-field disturbed zone and the far field, as shown in the lower left of Figure 4.3.4-1. Results are given in *Seepage Calibration Model for PA Including Drift Collapse* (CRWMS M&O 2000 [DIRS 153314], Tables 4 to 8).

Extended Rock Failure at the Drift Roof–Over time, extended rock failure may also occur at the roof of the drift. Kaiser (Brekke et al. 1999 [DIRS 119404], pp. D-11, D-12) estimated the failure at the roof to be 0.1 to 1 m in depth, or 0.4 to 1.2 m in depth if seismic effects were included. Generally, Kaiser expected that stress-induced failure at the drift crown would occur to a depth of half the drift radius (i.e., about 1.375 m). *Drift Degradation Analysis* (CRWMS M&O 2000 [DIRS 151554], Figures 39 to 40) used a discrete region key-block analysis that shows a more extended failure region, up to one drift radius above the drift ceiling. In the seepage study, a case is designed in which an extended cavity is found in the drift roof with a step shape of 0.5 m at the crown, 1 m depth at 0.5 m to one side, and so on, reaching 3 m depth at 2 m laterally from the drift crown (Figure 4.3.4-1, lower right). This shape is similar to that shown as a worst-case profile in *Drift Degradation Analysis* (CRWMS M&O 2000 [DIRS 151554], Figure 40). The step-shaped failure is 1 m thick.

Table 4.3.4-1 presents the calculated seepage percentages for Set A for three stochastic realizations (R1, R2, and R3) with drift degradation modes as defined in Figure 4.3.4-1, and compares them with the no-degradation case. (Seepage percentage is defined as the ratio of liquid that seeped into the drift to the total liquid arriving on a cross-sectional area corresponding to the footprint of the drift.) Only the cases where the percolation flux (Qp) is 500 mm/yr are shown in the table. This is the greatest value for which seepage percentages were calculated; it is four times as great as the simulated percolation under a glacial climate (CRWMS M&O 2000 [DIRS 153314], Section 6.3.7). The results show that the effect of a single rockfall is not significant for seepage. A deeper rock failure in the drift roof increases seepage. Calculations were also made with Set B, resulting in zero seepage for all cases, with or without drift degradation.

Additional simulations were done for other Q_p values to explore the effect of drift degradation on seepage threshold. The seepage threshold is a specific percolation flux at which seepage occurs. Figure 4.3.4-2 shows the calculated seepage percentage as a function of percolation flux Q_p for realization R3. It is seen in this figure that the effect of drift degradation for the three scenarios as defined above decreases with decreasing Q_p, so its impact on seepage threshold is relatively small. This can perhaps be explained by the fact that, under vertical percolation flux in a heterogeneous medium, the seepage threshold depends significantly on the horizontal cross section (footprint) of the drift. If the cross-sectional area does not change much, the seepage threshold will also not change much.

4.3.4.4 Developments Since Revision 01 of the Analysis Model Report

The previous studies, as described in Section 4.3.4.3 above, show that the extended rock failure case causes the largest impact on seepage. A more quantitative evaluation is presented in this section. Instead of the schematic rock failure profile shown in Figure 4.3.4-1, detailed degraded drift profiles calculated using a discrete region key-block analysis (DTN: MO0010RDDAAMRR.002 [DIRS 154048]) were used. The key-block analysis provides the following detailed three-dimensional drift profiles for seepage simulations, using a 0.305-m grid size.

For the Tptpmn unit:

1. Worst degradation (largest rockfall volume) profile
2. Profile at 75th percentile
3. No degradation (91.9 percent).

For the Tptpll unit, Set B′:

1. Worst degradation (largest rockfall volume) profile
2. Profile at 75th percentile
3. No degradation (99.6 percent).

For the Tptpmn, 91.9 percent of the drift length exhibits no drift degradation. Of the 8.1 percent that does exhibit degradation, the 75th percentile means that 75 percent of the 8.1 percent has a rockfall volume less than that shown in the 75th percentile drift profile. Similarly for Tptpll, 0.4 percent (100 percent to 99.6 percent) of the drift length exhibits drift degradation, with the 75th percentile profile indicating that 75 percent of 0.4 percent of the drift length has a rockfall volume that is less than that shown.

A typical example of the detailed degraded drift profile is shown in Figure 4.3.4-3 for the worst degradation profile in the Tptpnm unit.

4.3.4.5 Results of Analysis

Table 4.3.4-2 presents the seepage percentages for Set A of the Tptpmn unit with drift degradation modes (worst degradation case and degradation at 75th percentile) and compares them with the no-degradation case. Three realizations of the heterogeneous fields were used in these calculations (R1, R2, and R3). Figure 4.3.4-4 shows the results for Realization R1 graphically.

A series of percolation flux values (up to 500 mm/yr) was used to explore the effect of drift degradation on seepage threshold. Figure 4.3.4-4 shows that the effect of drift degradation for the scenarios decreases with decreasing Q_p, so its impact on seepage threshold is relatively small.

The results also indicate that seepage enhancement due to rockfall ranges from 0 to 5 percentage points for Q_p up to 500 mm/yr, owing to drift degradation for the worst case and 75th percentile case. The enhancement does not seem to depend on whether it is the worst case (i.e., the largest rockfall) or 75th percentile. These results suggest that the shape of the cavity in the ceiling may be more important for seepage enhancement than the volume. Confirming calculations were performed by using a homogeneous medium, and they also show more seepage for the 75th percentile case (Bodvarsson 2001 [DIRS 154669], Attachment 2, pp. 51 and 52).

Table 4.3.4-3 presents the seepage percentages for Set B′, representing the lower lithophysal unit, with drift degradation modes (worst degradation case and degradation at 75th percentile) and compares them with the no-degradation case. Here, because of the low seepage, values of Q_p up to 2,500 mm/yr were used. Three realizations of the heterogeneous fields were used in these calculations (R1, R2, and R3). Figure 4.3.4-5 shows the results for Realization R1 graphically. The results show that the seepage threshold is not significantly affected by drift degradation in the Tptpll unit; the enhancement is two percentage points or less.

Calculations with Set B parameter values resulted in zero seepage for all cases with percolation flux up to 2,500 mm/yr, with or without drift degradation (Bodvarsson 2001 [DIRS 154669], Attachment 2, p. 51).

4.3.4.6 Abstraction for Total System Performance Assessment

Seepage Model for PA Including Drift Collapse (CRWMS M&O 2000 [DIRS 153314], Section 6.6.4) showed that drift degradation tends to increase seepage. Seepage was consequently modeled for a few schematic degraded drift profiles. In the TSPA seepage abstraction, the worst of those modeled cases (Figure 4.3.4-1, lower right) was used for a conservative estimate of the possible effect of drift degradation on seepage. Compared with results presented in *Seepage Model for PA Including Drift Collapse* (CRWMS M&O 2000 [DIRS 153314], Sections 6.6.1, 6.6.2, and 6.6.3), the final estimate in the TSPA seepage abstraction included a 50 percent increase in seep flow rate to account for the potential effects of both drift degradation and degraded rock bolts (CRWMS M&O 2001 [DIRS 154291], Section 6.4.1). Rock bolt effects are examined in Section 4.3.3, in which it is concluded that rock bolts do not significantly increase seepage into emplacement drifts. Also, it will be shown here that the previous treatment of drift degradation effects in *Seepage Model for PA Including Drift Collapse* (CRWMS M&O 2000 [DIRS 153314], Section 6.6.4) was conservative.

Since the reporting of the abstractions used in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]), additional simulations of seepage for degraded drift profiles have been performed for drifts in the Tptpmn and Tptpll units and for a range of percolation fluxes (Bodvarsson 2001 [DIRS 154669], Attachment 2, pp. 51 to 54). The discussion in Sections 4.3.4.4 and 4.3.4.5 includes these new results, along with the simulations presented in the *Drift Degradation Analysis* (CRWMS M&O 2000 [DIRS 151635], Section 6) and included in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246], Figure 3.2-15). Note that the earlier work (CRWMS M&O 2000 [DIRS 153314], Section 6.6.4) used schematic degradation profiles with a uniform third dimension (parallel to drift axis) (i.e., a constant thickness in this direction). This is a simplification, from which no uncertainty range was calculated, and hence TSPA seepage abstraction used a 50 percent increase to account for potential effects of both drift degradation and degraded rock bolts (CRWMS M&O 2001 [DIRS 154291], Section 6.4.1). In the additional simulations presented here, this simplification was removed by using three-dimensional degradation profiles from *Drift Degradation Analysis* (CRWMS M&O 2000 [DIRS 151635]). This is a major step in reducing conceptual uncertainty. The new results show that compared to the no-degradation case, average seepage over the realizations in the Tptpmn unit (Set A) increased by 29 percent for the worst-case drift degradation and by 63 percent for the 75th percentile drift degradation at 500 mm/yr percolation flux (see Table 4.3.4-2). At 213.4 mm/yr percolation flux, the worst-case drift degradation increased average seepage by 17 percent, while the 75th percentile drift degradation increased seepage by a factor of about 6. For the lower lithophysal unit (Set B′), the seepage increase was greater for the worst-case drift degradation, with seepage increasing by or a factor of 2 to 3 for percolation flux ranging from 1,500 to 2,500 mm/yr. In addition, the seepage threshold decreased slightly: the worst-case degradation simulation showed a small amount of seepage at 1,000 mm/yr, whereas the base case had no seepage at that percolation flux.

These results must be put in perspective. As indicated in Section 4.3.4.4, no drift degradation occurred in 91.9 percent of the Tptpmn total drift length and in 99.6 percent of the Tptpll total drift length. Furthermore, most locations experiencing drift degradation had much less than the cases modeled here (75 percent of the locations with degradation had less degradation than the

75th percentile case). Thus, according to this analysis, a significant increase in seepage resulting from drift degradation would be relatively rare.

This increase in seepage at so few locations would not likely affect the overall average seepage. For example, take the largest increase mentioned above, an increase in seepage by a factor of 6 at 213.4 mm/yr for the Tptpmn unit. This increase applies to less than 8.1 percent at most, and probably less than 4 percent, of the locations (considering the 50th percentile drift degradation to have a much smaller effect on seepage). Thus, the increase in mean seep flow rate would be less than $0.04 \times 6 = 0.24$, or 24 percent. Since all the other calculated seepage increases were much less than a factor of 6, the increase in mean seep flow rate from drift degradation is likely much less than 24 percent. Furthermore, the effects would be even smaller for the lower lithophysal unit because the drift degradation analysis indicates less degradation in that unit and the seepage analysis indicates less seepage increase in that unit.

The results show that the impact on seepage calculated with this three-dimensional degradation profiles at different probability percentiles is similar to the result of the schematic profile, and the range is within the range used in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246], Section 3.2.4). In addition, the calculated seepage increases are small enough that they are well within the ranges of variability and uncertainty in seepage, as determined in the seepage abstraction for the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]). Thus, it appears that it is not necessary to increase the estimated seepage to account for drift degradation effects. Coupled with the finding in Section 4.3.3 that it is not necessary to increase the estimated seepage to account for rock bolt effects, it can be concluded that the seepage abstraction could be used for the TSPA model without the increase that was applied to account for drift degradation and rock bolts. That is, Table 13 of *Abstraction of Drift Seepage* (CRWMS M&O 2001 [DIRS 154291]) could be adapted for use rather than Table 16 of the same report. However, the TSPA analysis for this report is not adjusted for the new information discussed above, because further simulations are underway to account for heterogeneity by using multiple realization evaluations to provide results for seepage abstraction. Nevertheless, the new analysis has removed certain conceptual uncertainties as related to drift degradation and also to rock bolt effects (see Section 4.3.3) and make the TSPA abstraction on these issues more defensible.

4.3.4.7 Multiple Lines of Evidence

Underground tunnels or cavities are subject to potential degradation conditions, such as permeability changes in the rock surrounding the opening. Rockfalls are also frequently observed. No significant enhancement in seepage resulting from such degradation has been reported, and in general, seepage into underground cavities in unsaturated rocks, if any, is found to be a very small fraction of percolation flux. As discussed in Section 4.3.1.7, examples include tunnels in Rainier Mesa 30 km northeast of Yucca Mountain (Wang et al. 1993 [DIRS 108839]), caves in the UZ of a fractured limestone bedrock near Altamira, Spain, and observations of seepage into sealed segments of the ESF and the ECRB Cross Drift at Yucca Mountain. The model is consistent with the information from these sources. Further discussion on multiple lines of evidence related to seepage is presented in Section 4.3.1.7.

4.3.4.8 Summary of Uncertainty and Its Treatment

The uncertainty about seepage enhancement resulting from drift degradation has been addressed by starting with a detailed conceptual model that accounts for capillary-barrier diversion (due to the drift) and channelized or focused flow (due to fracture continuum heterogeneity). The parameter values needed for the simulations are based on those derived in the seepage calibration model using field data from the Tptpmn and Tptpll units. Finally, detailed drift degradation shapes obtained in the regional key-block analysis of field fracture data in the two units were used. For each of the two units, three cases were taken: (1) a no-degradation case, (2) a 75th percentile case, and (3) a worst case (i.e., largest rockfall volume). Simulations of seepage were performed for a series of percolation fluxes. For each case, three realizations of the heterogeneous field were used to account for geostatistical variations. Results indicate that seepage threshold is not affected by drift degradation and that seepage enhancement over a percolation flux up to 200 mm/yr for Tptpmn and 2,500 mm/yr for Tptpll units are about 5 percentage points or less. Table 4.3.4-4 summarizes uncertainty issues related to drift degradation and how they are addressed.

4.3.4.9 Summary and Conclusions

Four scenarios of detailed degraded drift profiles in the Tptpmn and Tptpll units, calculated using a discrete region key-block analysis (CRWMS M&O 2000 [DIRS 151635]), were selected for seepage calculations. Two types of drift degradation with implications for seepage enhancement have been examined: dilation and rockfall, with dilation effects having been previously considered.

Both rockfall and extended rock failure effects have been analyzed. The model has been refined over previous studies by use of a three-dimensional key-block analysis (replacing prior schematic two-dimensional rock failure profiling) and by incorporation of a revised set of calibrated mean parameters for the Tptpll.

Results in this section are based on seepage calibration model results (CRWMS M&O 2001 [DIRS 153045], Section 6.3.3 and 6.4.3). As more data from these units are obtained, parameter values with their uncertainties and probability weightings can be developed, allowing the seepage percentages presented in Section 4.3.4.6 to be used in performance assessment to obtain the best estimates (with uncertainty ranges) for use at Yucca Mountain. Uncertainty associated with geostatistics is evaluated through calculations of three realizations. Results for each case are shown in Tables 4.3.4-2 and 4.3.4-3. The spread of results from the three realizations gives an indication of geostatistical variation.

In summary, this section demonstrates that the impact of drift degradation and heterogeneity of the flow field can be evaluated. Generally, for both the Tptpmn and Tptpll units, simulated seepage enhancement due to drift degradation is calculated to be relatively small, with larger effects for larger percolation flux (Q_p) values. Seepage enhancement is between 0 and 5 percentage points in all three realizations, and less than 2 percentage points for the Tptpll. The enhancement does not seem to depend on whether it is worst case (i.e., largest rockfall) or 75th percentile. Seepage threshold was unaffected in almost all cases. The shape of a drift cavity created by rockfall may be more important to drift seepage than the volume of rockfall.

The current analysis has removed the conceptual uncertainty of schematic drift degradation profile by using calculated three-dimensional degradation profiles from the drift degradation analysis at different probability percentiles. This has made the TSPA uncertainty ranges used more defensible.

4.3.5 Thermal Effects on Seepage

4.3.5.1 Introduction

This section summarizes the modeling and uncertainty studies performed to determine the effects of heat on seepage of liquid water into emplacement drifts. The preceding sections discuss how, at ambient preemplacement conditions, the emplacement drift acts as a capillary barrier to divert water around the drift opening, and how seepage fluxes are lower than percolation fluxes. Analysis of seepage under ambient conditions emphasizes factors that determine whether water reaching the drift wall will actually seep into the drift. In this section, the focus is on how the thermo-hydrologic (TH) coupled processes affect the magnitude and spatial distribution of the percolation flux in the vicinity of the drift, since the percolation flux is the controlling factor for determination of seepage potential.

Modeling studies discussed in this section include alternative thermal operating modes for below-boiling and above-boiling temperatures within the rock mass as well as fracture heterogeneity, which has been shown to promote seepage (Tsang et al. 1997 [DIRS 100186]; Nitao 1997 [DIRS 100641]). As a result of these modeling and uncertainty studies, a more realistic abstraction for the TSPA is recommended. Thermal seepage models, as with any other models, are subject to uncertainties because of various factors, such as data, parameters, conceptualization, and numerical model implementation. A key issue for thermal seepage is the parameter uncertainty of different thermal operating modes and the effect of lithophysal cavities on thermal conductivity and heat capacity. Model implementation of the drift and discretization around the drift contribute to numerical model uncertainty. Perhaps the most important conceptual model uncertainty issue pertaining to thermal seepage is heterogeneity in important fracture parameters. Because of the limitation of data for coupled processes, the treatment of uncertainties must primarily be addressed by sensitivity studies. The uncertainty issues and their treatment are summarized in Section 4.3.5.8.

4.3.5.2 Goal of Thermal-Hydrologic Model for Seepage

The TH models presented in this section are intended to provide insight into how decay heat from emplaced waste will affect the magnitude and spatial distribution of percolation flux reaching the emplacement drifts and affect the potential for seepage into the drifts. The effect of TH processes on seepage is considered for the higher-temperature operating mode (HTOM) and the lower-temperature operating mode (LTOM). The results from these models will be used in a TSPA abstraction.

4.3.5.3 Mountain-Scale Coupled Process Model

4.3.5.3.1 Discussion of Revision 00 Results

Effects of repository heat on seepage into the drift were deduced indirectly from results presented in *Mountain-Scale Coupled Processes (TH) Models* (CRWMS M&O 2000 [DIRS 144454]). This model evaluates the effects of heat on UZ flow and distribution of liquid and temperature over a period of 100,000 yrs. The effect of climate was accounted for by applying the present-day infiltration rate for the first 600 yrs, followed by monsoon infiltration from 600 to 2,000 yrs and by glacial-transition infiltration thereafter. By necessity, numerical gridblocks used in three-dimensional flow modeling at the mountain scale are relatively large. To resolve the flow in the vicinity of the potential emplacement drifts, additional TH simulations were carried out for two-dimensional cross sections NS#1 and NS#2 (CRWMS M&O 2000 [DIRS 144454], Figure 1), with locally refined numerical grids to explicitly represent each 5-m diameter emplacement drift. The two-dimensional cross sections run approximately from the north to the south of the repository footprint, with the numerical discretization such that there are two or four lateral gridblocks (for NS#1 and NS#2 cross sections, respectively) between two adjacent emplacement drifts spaced at 81 m.

Because the primary objective of *Mountain-Scale Coupled Processes (TH) Models* (CRWMS M&O 2000 [DIRS 144454]) was to evaluate the effects of heat on mountain-scale flow, simulations were designed specifically to address large-scale flow issues relating to faults, perched water bodies, stratigraphic interface of the repository Topopah Spring unit with the upper Paintbrush and the lower Calico Hills units, etc. Therefore, the discussion about the effect of heat on potential seepage into the drifts is brief. Conclusions on thermal seepage were derived mainly from the simulated results from NS#2. This north-south section encompasses potential emplacement drifts located in different subunits of the Topopah Spring welded tuff, including the middle nonlithophysal and the lower lithophysal unit. The applied thermal load of 72.7 kW/acre for the three-dimensional mountain-scale numerical simulations translates to a line load of 1.45 kW/m in the two-dimensional simulations where the emplacement drifts are explicitly modeled. Forced ventilation for the first 50 yrs effectively removes 70 percent of the decay heat generated by the emplaced waste (Wilkins and Heath 1999 [DIRS 104247]).

Simulation results show that maximum temperatures occur in the drifts and minimum temperatures occur in the pillars between adjacent drifts. The temperatures in the pillars are predicted to rise to an average of 80° to 85°C. Temperatures rise to boiling in the immediate vicinity of the drifts, but may reach 110°C in drifts where ambient percolation flux is lower than average because of spatially variable infiltration. The dryout in both the fracture and matrix around the drifts is maintained for hundreds of years. Above the dryout zone are zones of increased liquid saturation, and large liquid flow rates (one to two orders of magnitude higher than the ambient flux) are predicted for the first one hundred years of emplacement, primarily through the fractures. The liquid fluxes toward the emplacement drift are driven by capillary pressure gradients resulting from the drying around the drifts. However, the ample decay heat from the potential emplacement drifts easily vaporizes this enhanced liquid flux, so in fact no liquid flux ever reaches the emplacement drift wall. That is, the coupled-process models predict no possibility for seepage when the temperatures in the rock mass around the drift are above boiling. This exclusion of liquid water is termed the "vaporization barrier." Vapor generated from the heat is driven away from the emplacement drift by pressure gradient, and subsequently condenses in cooler rocks and can drain down in fractures. Simulations predict that the drainage of thermally induced liquid flux through the pillars between the emplacement drifts mostly continues at a rate close to the ambient percolation flux for the thermal period, when temperatures in the rock mass remain above ambient.

4.3.5.3.2 Development since Revision 00

The work in *Mountain-Scale Coupled Processes (TH) Models* (CRWMS M&O 2000 [DIRS 144454]) was based on the Enhanced Design Alternative (EDA) II repository design, which specifies an initial thermal load of 72.7 kW/acre (1.45 kW/m of drift) and a forced ventilation period of 50 yrs, during which 70 percent of the decay heat is removed (Wilkins and Heath 1999 [DIRS 104247]). The thermal load of EDA II (Wilkins and Heath 1999 [DIRS 104247]) gave rise to above-boiling temperatures in the rocks in the vicinity of the emplacement drifts for hundreds of years. The EDA II thermal impact is referred to as the higher-temperature case. Model development since the higher-temperature case documented in the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) involves studies of coupled processes for a range of temperatures.

In the lower-temperature options, the rock temperature does not go above boiling anywhere in the repository. In the LTOM, an initial thermal load of 67.7 kW/acre (1.35 kW/m of drift) and a forced ventilation period of 300 yrs (during which 80 percent of the heat is removed) are applied.

Model development since *Mountain-Scale Coupled Processes (TH) Models* (CRWMS M&O 2000 [DIRS 144454]) also focuses on assessing uncertainties pertaining to thermal seepage, particularly for potential emplacement drifts in the lower lithophysal unit (where more than 70 percent of the potential repository would be located). As heterogeneity is known to promote flow channeling and fast flow that can enhance seepage, small-scale heterogeneity in the fracture properties is incorporated. The approach of Monte Carlo simulations is taken in order to investigate whether the general conclusions continue to hold—that no liquid flux can penetrate the vaporization barrier of the higher-temperature repository and reach any drift. Also, studies are being carried out to determine whether a vaporization barrier to prevent downward-percolating liquid flux from seeping into the emplacement drift would also exist for a lower-temperature repository operating mode.

All model developments since *Mountain-Scale Coupled Processes (TH) Models* (CRWMS M&O 2000 [DIRS 144454]) are documented in Bodvarsson (2001 [DIRS 154669], Attachment 6, pp. 24 to 51, and Attachment 17, pp. 39 to 75).

Specifically, these developments include:

1. Refinement of numerical model grids in all subunits of the Topopah Spring welded tuff. Instead of studying flow effects on all potential emplacement drifts in NS#2, this model concentrates on only one emplacement drift in NS#2, located in the lower lithophysal unit. The lateral boundary of the model extends to the midpoint between two adjacent drifts at 40.5 m from the center of the emplacement drift. The refined grids allow for better resolution of the distribution of percolation flux in the vicinity of

an emplacement drift than the Rev 00 AMR results, which are based on coarse grids (two or four lateral gridblocks between two potential adjacent drifts).

2. Incorporation of small-scale heterogeneity in the fracture permeability, with values ranging over four orders of magnitude (based on air-permeability measurements in boreholes in the ESF and the ECRB Cross Drift) (DTN: LB0011AIRKTEST.001 [DIRS 153155], DTN: LB0012AIRKTEST.001 [DIRS 154586], DTN: LB002181233124.001 [DIRS 146878], DTN: LB980901233124.004 [DIRS 105855], DTN: LB980901233124.001 [DIRS 105821], DTN: LB980912332245.001 [DIRS 110828]). The random heterogeneous fields are superposed on the $1 \text{ m} \times 1 \text{ m}$ gridblocks around the drift (measurements do not show any spatial correlation larger than the size of the gridblock).

3. Inclusion of a discrete high-permeability feature that intersects the emplacement drift, in addition to the heterogeneous fracture permeability field in the repository unit. This is intended for studying the competing processes of fast drainage in a preferential path to the drift and the vaporization potential of that liquid drainage flux due to the waste heat.

4. Exercising of models with items (1) through (3) above using the same hydrological and thermal properties for the lithophysal units as in the AMR for the above-boiling operation mode.

5. Exercising of models with items (1) and (2) above using the thermal conductivity and heat capacity of the rock mass, which accounts for the lithophysal porosity of the upper and lower lithophysal units in the matrix properties for the HTOM and LTOM.

In *Mountain-Scale Coupled Processes (TH) Models* (CRWMS M&O 2000 [DIRS 144454]), the thermal-conductivity and heat-capacity parameters used were based on laboratory core measurements. Mapping data along the ECRB drift walls (Mongano et al. 1999 [DIRS 149850], Figures 2 and 3) indicate that the mean lithophysal porosity, ϕ_L, of the upper and lower lithophysal units is 0.216 and 0.125, respectively. Since the thermal conductivity (λ) of air is almost 2 orders of magnitude smaller than that of rock and 20 times smaller than that of water, the bulk thermal conductivity of the lithophysal units would be lower if the lithophysal porosity were explicitly accounted for. Applying a parallel model to incorporate the lithophysal porosity, the bulk rock thermal conductivity becomes the weighted average:

$$\lambda_{\text{with lithophysae}} = \lambda_{\text{matrix}} (1 - \phi_L) + \lambda_{\text{air}} \phi_L \qquad \text{(Eq. 4.3.5-1)}$$

Implicit in Equation 4.3.5-1 is that the lithophysal cavity is always air-filled, regardless of whether the thermal-conductivity measurements were made on "wet" matrix cores (where the matrix porosity is 100 percent water-filled) or on "dry" matrix cores (where the matrix porosity is air-filled). This is reasonable because the capillary barrier effect noted earlier also acts to exclude water from the lithophysae, even if the matrix is saturated.

The rock grain heat capacity C_R was similarly modified to account for the effect of lithophysal porosity on heat conduction in the matrix continuum, according to:

$$C_R^* = C_R (1- \phi_m - \phi_L)/ (1- \phi_m) \qquad \text{(Eq. 4.3.5-2)}$$

where ϕ_m is the matrix porosity.

A comparison of parameter values for the thermal properties used in *Mountain-Scale Coupled Processes (TH) Models* (CRWMS M&O 2000 [DIRS 144454]) to the developments since issuance of the AMR, which included lithophysae effects on thermal properties, is presented in Table 4.3.5-1.

4.3.5.3.3 Results of Analysis since Revision 00

All model developments since *Mountain-Scale Coupled Processes (TH) Models* are documented in Bodvarsson (2001 [DIRS 154669], Attachment 6, pp. 24 to 51, and Attachment 17, pp. 39 to 75). As discussed in Section 4.3.5.3.2, simulations of flow in the vicinity of one emplacement drift in the lower lithophysal unit were carried out for different realizations of fracture heterogeneity. Presence of lithophysal cavities gives rise to uncertainty pertaining to TH effects on seepage. These gas-filled cavities modify the thermal properties of the rock matrix from those in the AMR, as outlined in Table 4.3.5-1. To resolve the uncertainty due to lithophysal properties on the TH processes, simulations using the lithophysae thermal property (Table 4.3.5-1) are compared with those using the property set (with no effect of lithophysae) in *Mountain-Scale Coupled Processes (TH) Models* (CRWMS M&O 2000 [DIRS 144454]). To illustrate, the time evolution of temperature at the drift wall using both the nonlithophysae and lithophysae property sets are shown in Figures 4.3.5-1a and 4.3.5-1b for the HTOM and LTOM, respectively. Note the sharp increase of temperature following cessation of forced ventilation at 50 and 300 yrs, respectively, in Figures 4.3.5-1a and 4.3.5-1b. In Figure 4.3.5-1a, another temperature increase occurs at dryout at about 80 yrs, when no more water is available to absorb the heat of vaporization. In both operating modes, the drift wall temperatures from the property set incorporating the effects of lithophysal cavities are at most 6 C° higher than the ones from the AMR property set. This indicates that lithophysal cavities do not significantly impact the temperatures. However, the possible impact of these gas-filled lithophysal cavities on thermally induced fluid flow in the fractures and the matrix, and the subsequent moisture redistribution, has not yet been investigated rigorously. This is a remaining uncertainty that could be resolved by new conceptual models and field measurements in the lithophysal unit.

A primary objective of the current studies is to determine whether fast-flow liquid flux promoted by fracture heterogeneity can penetrate the vaporization zone around a potential emplacement drift. Monte Carlo studies (Bodvarsson 2001 [DIRS 154669], Attachment 6 and 17) show that even with the incorporation of fracture heterogeneity (based on field measurements), results similar to those in the AMR for homogeneous fracture property are obtained. That is, even though substantial enhancement in the fracture fluxes does occur at several meters above the drift, these enhanced liquid fluxes do not reach the drift crown during the thermal period. In Figure 4.3.5-2, fracture liquid fluxes as a function of lateral distance from the center of the drift are plotted for two horizontal lines at different times since waste emplacement. In Figure 4.3.5-2a, the fracture liquid fluxes are shown at an elevation of 5 m above the top of the drift. It is clear that fluxes exceed the ambient infiltration rate (about 4.8 mm/yr for present day until 600 yrs after waste emplacement), especially 100 yrs after waste emplacement. The enhanced fluxes result from the increased fracture saturation in the condensation zone and capillary suction toward the dryout zone. In Figure 4.3.5-2b, the fluxes are shown for the elevation of the drift horizon. Here, it is evident that none of the enhanced fluxes can cross the drift horizon within the drift. On the other hand, Figure 4.3.5-2b shows drainage fluxes in the pillars beyond the drift wall, which is at 2.5 m from the drift center. The drainage flux moves out laterally with time because of the drying around the drift.

Figure 4.3.5-2 is typical of simulations with different realizations of the heterogeneous permeability field for the higher-temperature case. Results from different realizations confirmed this phenomenon of enhancement of fracture fluxes several meters above the drift from the condensation, and reduction (often to zero) of fracture fluxes below the condensation zone, both above and below the drift. Maximum thermally enhanced liquid fluxes occur about 100 yrs after emplacement. However, the evaporative energy of decay heat for the above-boiling operating mode appears to be effective in keeping liquid water from reaching the emplacement drift. Thus, for the HTOM, where above-boiling temperatures occur around the emplacement drift, simulated results show that fracture fluxes would not likely seep into the drift.

Contour plots of liquid saturation show the moisture redistribution and give insight to thermally induced distribution of liquid flow. Zones of increased liquid saturation usually lead to higher liquid fluxes, and vice versa. Figures 4.3.5-3a and 4.3.5-3b show contours of liquid saturation in the fractures around an emplacement drift at 50 and 100 yrs after emplacement of radioactive wastes for the higher-temperature case. The thermal property set that incorporates the effects of lithophysal cavities, as described in Table 4.3.5-1, is used in these simulations. Figure 4.3.5-3a shows that at 50 yrs, a dryout has formed below the emplacement drift; however, there is no perceptible dryout zone above or lateral to the drift. Figure 4.3.5-3b shows that at 100 yrs after waste emplacement, the extent of the dryout zone has increased considerably. A pattern of considerably larger drying below the drift (rather than above or to the side of the drift) persists. This phenomenon of a "dry shadow" below the drift can significantly impact transport, as discussed in Section 11.3.5. Because of the underlying small-scale heterogeneities in the permeability field, localized zones of condensate accumulation appear. This is in contrast to the continuous condensate zone in simulations with a uniform permeability distribution. The liquid saturation in the condensate-zone fractures can increase to 5 percent from the ambient values of 1 to 1.5 percent. This increased saturation beyond the dryout zone laterally results in drainage through the cooler region between two adjacent emplacement drifts. These phenomena of drying and wetting continue past 1,000 yrs after waste emplacement. Throughout this period, the extent of the dryout zone does not exceed 10 m above the drift or 15 m laterally. Below the drift, however, the dryout zone extends down to a maximum of 60 m. Simulated results for different realizations of permeability fields produce similar patterns, with only minimal variations in the extent of dryout zones and the amount of condensate build-up.

The drying around the emplacement drift resulting from vaporization in a HTOM is also illustrated in a contour plot of liquid saturation in the matrix. Figure 4.3.5-4 shows the liquid saturation distribution in the matrix at 1,000 yrs after emplacement (Bodvarsson 2001 [DIRS 154669], Attachment 6, p. 37). Note the large decrease of the liquid saturation from ambient (about 0.9) to less than 0.01 and the extent of the drying.

Since none of the simulations with stochastic permeability fields led to seepage during the thermal period for the higher-temperature case, one stochastically generated permeability field was modified: the permeability of a column of fracture elements intercepting the drift crown was artificially increased by a factor of 100 to investigate the impact of a high-permeability discrete feature, such as a fault, on thermal seepage. The simulated results are shown in Figure 4.3.5-5. Again, fracture liquid fluxes are plotted as a function of lateral distance from the center of the drift for a horizontal line at the drift elevation and at different times since waste emplacement. Figure 4.3.5-5 shows that no liquid flux can cross the drift horizon within the drift up to 1,000 yrs after emplacement, and that there is enhancement of drainage flux beyond the drift. The small "ambient" flux shown within the drift at 0.01 yrs is an artifact of the numerical model: in this particular simulation, the drift has not been modeled as a capillary barrier, but has nonzero capillary suction that can draw water at the initial drying. However, the thermal effect quickly overcomes this artifact: Figure 4.3.5-5 shows no seepage into the drift throughout the thermal period of 1,000 yrs, even for this case of an artificial high-permeability discrete feature intersecting the drift at the center line.

Similar Monte Carlo simulations were carried out for the lower-temperature case (Bodvarsson 2001 [DIRS 154669], Attachment 6 and 17). As expected, the simulated results show smaller thermal perturbation around the emplacement drift compared to the higher-temperature case. Figure 4.3.5-6 shows the temperatures at the emplacement drift wall as a function of time (logarithmic scale) for both operating modes. The figure also includes a third lower-temperature scenario with 300 yrs of forced ventilation and an initial thermal load of 1.45 kW/m. The higher-temperature case predicts a maximum drift wall temperature of approximately 120°C, whereas the maximum drift wall temperature for the LTOM is about 84°C with a heat load of 1.35 kW/m, or 88°C with a heat load of 1.45 kW/m. All these results were obtained through simulations using the lithophysae thermal property set listed in Table 4.3.5-1. Note that, because temperatures are gridblock averages, simulated drift-wall temperatures will increase with refinement of the numerical grid.

The higher-temperature case predicts a maximum drift wall temperature of approximately 120°C, whereas the maximum drift wall temperature for the LTOM is about 84°C with a heat load of 1.35 kW/m, or 88°C with a heat load of 1.45 kW/m. All these results were obtained through simulations using the lithophysae thermal property set listed in Table 4.3.5-1. Note that, because temperatures are gridblock averages, simulated drift-wall temperatures will increase with refinement of the numerical grids.

Since the smaller thermal perturbation from the lower-temperature case produces no boiling anywhere in the rock, there is minimal redistribution of moisture. If the contours of matrix liquid saturation were plotted on the same scale as that in Figure 4.3.5-4 for the higher-temperature case, little reduction of liquid saturation from the ambient value would be observed anywhere at any time after emplacement.

A far smaller amount of water resides in the fractures (the pore volume of the fracture continuum is at least an order of magnitude smaller than that of the matrix, and the ambient liquid saturation in the fractures is about two orders of magnitude smaller than in the matrix). Hence, contours of liquid saturation in the fractures will be more sensitive to the small heat perturbation of the lower-temperature case. The thermal perturbation of the lower-temperature case can produce some drying below the emplacement drift in the fractures. Even below boiling, vapor pressure increases with increased temperature, reducing the amount of water in the liquid phase. Figures 4.3.5-7a and 4.3.5-7b show the fracture liquid saturations from the lower-temperature case at 50 and 500 yrs after emplacement. Note that Figure 4.3.5-7a shows a slight increase in saturation immediately above the square drift. This results from ponding of downward flux on the drift top, since the drift is modeled as a capillary barrier with zero capillary suction. Decay heat to the rock increases when forced ventilation ceases at 300 yrs, so at 500 yrs the drying in the fracture extends downward to about 40 m. The drying is absent above and to the side of the drift because the effect of downward percolation flux and shedding to the side of the drift (which acts as a capillary barrier) more than compensates for the small amount of drying in the fractures due to vaporization. For the same reason, Figure 4.3.5-7 shows no localized zones of condensate build-up, as seen in Figure 4.3.5-3 for the higher-temperature case.

Because the temperatures are below boiling for the lower-temperature case, a great enhancement of percolation flux from ambient values would not be expected above the drift. This is confirmed by Figure 4.3.5-8a, where the fracture liquid fluxes at 5 m above the top of the drift are plotted as a function of lateral distance from the center of the drift at different times since emplacement (compare with Figure 4.3.5-2a). In Figure 4.3.5-8b, the fracture liquid fluxes are plotted at the drift center horizon. The drift acts as an effective capillary barrier so that no liquid flux enters the drift. Rather, it sheds around the drift, giving rise to an increased liquid flux immediately outside the drift wall at 2.5 m.

The results described above indicate that on one hand the TH coupled processes of boiling and condensation in the HTOM increase uncertainties associated with the movement of water; on the other hand, the presence of the vaporization barrier when temperature is above boiling quite certainly prevents percolation flux from reaching the drift wall, reducing the uncertainties associated with seepage into the drift compared to the LTOM.

4.3.5.4 Multiscale Thermal-Hydrologic Model

4.3.5.4.1 Discussion of Revision 00 Results

The *Multiscale Thermohydrologic Model* (CRWMS M&O 2000 [DIRS 149862]) is used primarily to develop time-varying estimates of key engineered barrier system performance measures (e.g., drift wall temperature, waste package temperature, relative humidity in the drift). These performance measures depend on TH behavior within a few meters of the emplacement drifts, and also on the scale of the repository (because of differences in local stratigraphy and local percolation flux). Thus, the multiscale thermal-hydrologic (MSTH) model takes a multiscale approach that combines one-dimensional, two-dimensional, and three-dimensional drift-scale thermal and TH models with a conduction-only three-dimensional mountain-scale model. Results of this show that over the entire range of the infiltration flux conditions considered, seepage is not predicted to occur during the boiling stage of the HTOM. After the cessation of boiling in the host rock (but not necessarily in the drift), seepage is predicted to occur only at a limited set of locations under high infiltration conditions. Under low to moderate infiltration conditions, no seepage into the drift is predicted to occur by the MSTH model. During the period in which boiling has ceased in the host rock but continues in the drift, seepage may occur under high infiltration conditions, but water entering the drift quickly evaporates.

Similar to the findings reported in Section 4.3.5.3.3, the MSTH model results show that at several meters above the drift crown, thermally induced percolation fluxes are greatly enhanced from their ambient values. However, these enhanced percolation fluxes are not able to penetrate the vaporization barrier to reach the drift wall.

Although the TH simulations in the MSTH model show no evidence of seepage during the boiling period (i.e., when temperatures are above boiling) for the HTOM (and little evidence of seepage during the below-boiling stage except under high infiltration conditions), the TSPA-SR (CRWMS M&O 2000 [DIRS 153246], Section 3.2.4) adopted a conservative approach, in which the increased percolation fluxes at 5 m above the drift crown calculated with the MSTH model were chosen as the seepage fluxes in the abstracted seepage model presented in *Abstraction of NFE Drift Thermodynamic Environment and Percolation Flux* (CRWMS M&O 2001 [DIRS 154594]). This conservative approach gives rise to an artificial peak in the abstracted seepage flow rates for all 610 locations within the heated repository footprint immediately after the forced ventilation period of 50 yrs. The justification for the conservative approach is partly based on the observation that the MSTH model uses a homogeneous fracture continuum within any given hydrostratigraphic unit (i.e., drift-scale heterogeneity is neglected), while drift-scale heterogeneity is known to promote focusing and channeling of flow.

4.3.5.4.2 Model Development since Total System Performance Assessment-Site Recommendation Investigating Heterogeneity

Drift-scale heterogeneity of fracture properties was incorporated into the three-dimensional heterogeneous line-averaged-heat-source, drift-scale thermal-hydrologic (LDTH) submodel of the MSTH model (BSC 2001 [DIRS 154985]). While REV 00 of the MSTH model demonstrates that seepage into the drift rarely occurs, it is possible that the very low occurrence of predicted drift seepage results partly from the modeling of a homogeneous fracture continuum within the host rock units. Since the issue of whether heterogeneity can increase the occurrence of liquid flux penetrating through a vaporization barrier is specific to above-boiling temperatures, the lower-temperature case is discussed in this subsection.

The three-dimensional heterogeneous LDTH models used are all based on the two-dimensional LDTH submodel at a location close to the geographic center of the repository. This location has infiltration fluxes that are higher than the repository averages for the present-day, monsoon, and glacial climates. A mean infiltration flux of 10.14 mm/yr for the first 600 yrs, 24.09 mm/yr from 600 to 2,000 yrs, and 38.66 mm/yr after that is modeled. The host rock unit at this location is the Tptpll. The three-dimensional LDTH model has a longitudinal dimension of 5 m (approximately the length of one waste package). Gridblock spacing in the longitudinal direction is 1.0 m. Capillary pressure and relative permeability are described by van Genuchten's function, with 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). The fracture porosity is correlated to the heterogeneous fracture permeability field according to the cubic law (Bear 1988 [DIRS 101379], p. 166). Random fields for heterogeneous fracture properties were generated by the Fourier spectral method in three dimensions (Nitao 1997 [DIRS 100641]) for the key fracture properties: permeability, porosity, and the van Genuchten "alpha" parameter. In the heterogeneous fracture field, fracture permeability values are isotropic, which is realistic. All stochastic realizations use a lognormal distribution with values of $\log_{10}$ standard deviation and correlation lengths in the principal directions (BSC 2001 [DIRS 154985], Table 6-8). Some of the stochastic realizations used a $\log_{10}$ standard deviation that is considerably greater than the value of 0.72 determined from air-permeability data gathered at ESF Niche 2 (Station 36+50) (CRWMS M&O 2000 [DIRS 141400], Table 5).

Eight separate stochastic realizations were considered (Table 4.3.5-2): four pertain to a center location in the repository (Cases A-56 to D-56) and four pertain to an edge location (Cases A-34 to D-34). Six of these realizations use a standard deviation larger than that derived from air-permeability measurements made in Niche 2 (Station 36+50) (CRWMS M&O 2000 [DIRS 141400], Figures 11 and 12). The larger values of $\log_{10}$ standard deviation were chosen to increase the focusing of liquid-phase flow, and thereby increase the likelihood of seepage into the drift. Case A is intended to examine the influence of a large correlation length in the vertical direction, as compared to the horizontal direction. This has the effect of focusing flow along vertically oriented heterogeneities, which increases the tendency for seepage. Case B was intended to investigate whether capillarity is correlated with permeability. Case C is considered to be a more realistic case in that there is no vertical biasing to the shape of heterogeneities, which is more consistent with gas-permeability measurements made in Niche 2 (Station 36+50), and the standard deviation for permeability used in the realization (1.0) is close to that derived from those measurements (0.72). Case D examines the influence of a large standard deviation in the permeabilities while using a moderate ratio of vertical to horizontal correlation length.

4.3.5.4.3 Results of the Analysis Investigating Heterogeneity

TH simulations with the three-dimensional LDTH model applied to heterogeneous fields show no seepage entering the emplacement drift during the boiling stage of the HTOM, even when using stochastic hydrologic parameters favoring seepage that are well outside of currently available distributions measured at the site. Hence, the conclusion that no seepage occurs during the boiling stage appears to be robust and is not altered by the incorporation of small-scale heterogeneity. These results are consistent with those presented in Section 4.3.5.3.3.

Figure 4.3.5-9 shows the influence of drift-scale heterogeneity of permeability on the distribution of percolation flux in the host rock for Realization C-56. The influence of three different climate states is readily apparent as three distinct steps in the percolation histories. Close to the drift wall, the influence of decay heat on local percolation flux is seen to occur in three stages: (1) an initial stage of thermally enhanced percolation flux, which is seen as a distinct spike just after 50 yrs; (2) a period in which rock dryout reduces percolation flux; and (3) a post-boiling period. During the early portions of the post-boiling period, percolation flux is enhanced (seen as a second spike at approximately 700 yrs) as a result of a residual condensate zone that developed earlier, during the boiling stage. Note that 700 yrs corresponds to the time when the boiling zone has receded past the location 3 m above the drift (Figure 4.3.5-9b). This relatively short-lived phenomenon (on the order of hundreds of years) is followed by a period where percolation flux is no longer influenced by decay heat. Figure 4.3.5-10 shows that although the distribution of percolation flux is heterogeneous, there is a negligible influence on the distribution of temperature and relative humidity in the host rock.

Because such extreme examples of heterogeneity were considered and a large number of realizations were not considered, it is not possible to use these calculations to determine the probability of seepage during the post-boiling period. However, these calculations are useful for making the following observations:

1. During the boiling period, seepage is extremely unlikely.

2. During the post-boiling period, the likelihood and magnitude of seepage increase with the $\log_{10}$ of the standard deviation of the fracture permeability.

3. During the post-boiling period, the likelihood and magnitude of seepage increase with the ratio of vertical to horizontal correlation length.

4. During the post-boiling period, 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.

5. The duration of the boiling period is never reduced as a result of fracture heterogeneity. In fact, 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, with the low-*k* features obstructing buoyant gas-phase convection. Thus, buoyant gas-phase convection plays a less significant role in the rate of cooldown in the drift for a heterogeneous case than for a corresponding homogeneous case.

6. During both the boiling and post-boiling periods, temperatures at the drift wall are insensitive to heterogeneity. Figures 4.3.5-9 and 4.3.5-10 show simulation results for the most realistic stochastic realizations considered (BSC 2001 [DIRS 154985], Cases C-56 and C-34, Table 6-8). These figures illustrate the effect of the vaporization barrier discussed in Section 4.3.5.6.1. In the simulation results shown in Figure 4.3.5-9, liquid water percolated downward 5 m above the drift crown, but 3 m above the drift crown, there was no percolation flux between approximately 60 and 340 yrs. Percolation flux was also zero in the interval between the drift crown and 3 m above the drift crown. The upper drift-wall temperature, shown in Figure 4.3.5-10, was above 100°C during this time. After the boiling period, these simulations produced no seepage due to diversion by capillary forces (BSC 2001 [DIRS 154985], Table 6-10).

4.3.5.5 Analytical Solution to Assess Liquid Fingering through a Superheated Regime

The possibility of large, randomly fluctuating infiltration rates caused by asperity-induced episodic flow through the fractures was considered. The analytical solution of Phillips (1996 [DIRS 152005]) was used to determine the penetration distance of the infiltration into the superheated fractured rock. Cumulative distribution functions for the episodicity and a critical penetration distance were developed to provide estimates for the probability of liquid water penetrating through the superheated region to a prescribed location.

The conceptual model governing asperity-induced episodic infiltration models fractures as consisting of randomly distributed "pinch-point" and "storage" apertures within the fractures. The pinch-point apertures act as capillary barriers to the infiltration of water, which accumulates in a volume above the pinch-point dictated by the storage aperture. The water continues to accumulate in the storage aperture until the head above the pinch-point aperture exceeds the associated capillary rise height. Once this happens, the water flows downward under the forces of gravity and at a rate dictated by the permeability of the aperture. The water continues to flow through the aperture until the accumulated water is completely drained. This behavior leads to an asperity-induced episodic infiltration of water through fractured rock that occurs randomly in space and time.

A region of superheated rock is modeled as existing below the source of asperity-induced episodic infiltration. The water percolates downward into the superheated rock and begins to boil. The rate of evaporation is dictated by the conductive heat transfer from the adjacent rock to the flowing water. The analytical solution of Philips (1996 [DIRS 152005]) is used to determine the penetration distance of the water into the superheated rock based on the flow rate, volume of water available for drainage, and heat transfer from the adjacent rock. Although the size of the liquid fingers (or "weeps") flowing down the fractures will be considered in three dimensions, the flow process is modeled as occurring in one dimension to facilitate an analytical solution.

The conceptual model described above consists of two primary processes: (1) the accumulation and drainage of water in fractures and (2) the penetration of that water into superheated rock. The sections below describe the mathematical models for each of these processes.

4.3.5.5.1 Accumulation and Drainage of Water in Fractures

The capillary rise height, h [m], in a fracture plane above the pinch-point aperture can be calculated using the Young-Laplace equation (Bear 1988 [DIRS 101379], p. 445):

$$h = \frac{2\sigma}{\rho g b_2} \qquad \text{(Eq. 4.3.5-3)}$$

where

σ = the surface tension of water [N/m]
ρ = the liquid density [kg/m^3]
g = the gravitational constant [9.81 m/s^2]
b_2 = the pinch-point aperture [m]

The maximum volume of water, V [m^3], that can be stored above the pinch-point aperture is expressed as a function of the capillary rise height:

$$V = hb_1 w \qquad \text{(Eq. 4.3.5-4)}$$

where

b_1 is the storage aperture ($b_1 > b_2$) and w is the width [m] of the ribbon or "finger" of water flowing along the fracture plane (the width, w, is measured in a direction perpendicular to the aperture).

When the accumulation of water in the storage aperture produces a head that exceeds the capillary rise height given by Equation 4.3.5-3, the water will flow through the pinch-point aperture. The mass flow rate, $\dot{m}_o$ [kg/s], can be determined by treating it as steady laminar flow between parallel plates separated by the pinch-point aperture (Bear 1988 [DIRS 101379], p. 166):

$$\dot{m}_o = \left[\frac{b_2^{\,2}}{12\mu} \rho g \right] \rho b_2 w \qquad \text{(Eq. 4.3.5-5)}$$

where

μ	=	the dynamic viscosity of water [kg/m-s]
kg/m-s	=	the flow velocity [m/s].

The time, t_d [s], required to drain the water through the pinch-point aperture can be calculated by dividing the total mass of accumulated water by the mass flow rate through the pinch-point aperture:

$$t_d = \frac{\rho V}{\dot{m}_o} \qquad \text{(Eq. 4.3.5-6)}$$

The mass flow rate (Equation 4.3.5-5) and the time required to drain the water (Equation 4.3.5-6) are used in subsequent calculations to determine the water-penetration distance into superheated rock. In addition, the episodicity of the water flowing through the fracture can be determined based on the duration of the accumulation and drainage processes. The episodicity factor, e, is defined as the ratio of the drainage time, t_d [s], to the accumulation time, t_a [s]. It represents the fraction of time that breakthrough flow occurs in a fracture experiencing asperity-induced accumulation and drainage. The accumulation time, t_a, can be expressed by dividing the maximum mass of accumulated water (as derived from Equation 4.3.5-4) by the mass flow rate of infiltrating water coming into the storage aperture:

$$t_a = \frac{\rho V}{\rho u A} \qquad \text{(Eq. 4.3.5-7)}$$

where

u	=	a Darcy infiltration flux rate [m/s] that can be specified by surface infiltration
A	=	a cross-sectional area representing a catchment region that collects and focuses water into the fracture.

The catchment area represents the bulk cross-sectional area associated with the Darcy velocity for each fracture that has flowing water. If the fingers of water flowing down the fractures are separated by a uniform "weep" distance, a, the cross-sectional area, A, can be expressed as a^2 (Ho and Wilson 1998 [DIRS 123261]). The episodicity factor, e, can then be expressed as follows:

$$e = \frac{t_d}{t_a} = \frac{\rho u A}{\dot{m}_o} \qquad \text{(Eq. 4.3.5-8)}$$

The episodicity factor is bounded by 0 (no flow) and 1 (always flowing). The drainage time may, in some cases, exceed the accumulation time, which yields a constant flow condition. In these cases, the maximum value of the episodicity factor is set equal to one. As an example, if the episodicity factor is equal to 0.1, flow drains through the fracture only one-tenth of the time. Over one year, percolation draining through this fracture would only occur approximately five weeks.

4.3.5.5.2 Water Penetration into Superheated Rock

Phillips (1996 [DIRS 152005]) developed an analytical model of infiltration into superheated fractured rock. A ribbon of liquid water is modeled as flowing down a fracture in an unsaturated rock matrix and boiling as it passes the boiling-point isotherm. The temperature in the superheated rock beyond the boiling-point isotherm is greater than the boiling temperature, but the temperature of the penetrating liquid remains at the boiling temperature. The penetration distance into the superheated rock is a function of the mass flow rate of liquid across the boiling-point isotherm, the heat conduction available from the surrounding rock, and the properties of the fluid and rock. The solution models the flow as one-dimensional and the heat flux and initial mass flow rate as constant. The penetration distance, l [m], derived by Phillips (1996 [DIRS 152005]) is given as:

$$l = \left(\frac{2}{\pi}\right)^{0.25} L_3 \left(\frac{\alpha t}{w^2}\right)^{0.25} \quad \text{for } t < w^2/\alpha \qquad \text{(Eq. 4.3.5-9)}$$

where

α	=	the effective thermal diffusivity of the rock matrix [m^2/s]
t	=	the duration of the infiltration event [s]
L_3	=	a characteristic length.

The characteristic length is defined as follows:

$$L_3 = \left(\frac{\dot{m}_o h_{fg}}{q}\right)^{0.5} \qquad \text{(Eq. 4.3.5-10)}$$

where

q = the heat flux available to boil the water penetrating into the superheated rock [W/m^2]

h_{fg} = the latent heat of vaporization [J/kg]

Phillips (1996 [DIRS 152005]) expresses this heat flux in terms of Fourier's Law (i.e., thermal conductivity multiplied by temperature gradient). The duration of the infiltration event, t, in Equation 4.3.5-9 is equal to the drainage time, t_d, which specifies a period of constant mass flow rate supplied to the superheated region, as required by the Phillips (1996 [DIRS 152005]) solution.

An energy balance on the evaporating ribbon of water specifies that the heat flux, q, is proportional to the rate of water evaporation. Therefore, Equation 4.3.5-10 can be interpreted as the ratio of the mass flow rate of water entering the superheated region to the mass rate of water being evaporated. If this ratio is large, then the penetration distance can be large because the mass flow rate is able to overcome the rate of evaporation. The characteristic length, L_3, in Equation 4.3.5-10 is also an approximate solution for the penetration distance when $t \geq w^2/\alpha$ (Phillips 1996 [DIRS 152005], pp. 1669 to 1670).

The downward flow rate at a location, z, in the superheated region can be derived from a mass balance between the downward flow rate and the mass rate of evaporation. The mass balance is given in Phillips (1996 [DIRS 152005], Equation 10) as follows:

$$\frac{\partial}{\partial z}[\dot{m}(z)] = -\left(\frac{8}{\pi}\right)^{0.5} \frac{q}{h_{fg}} \frac{z}{\left[\alpha w^{-2}(t - t_z)\right]^{0.5}} \text{ for } t_z < t < w^2/\alpha \qquad \text{(Eq. 4.3.5-11)}$$

where

z = the distance below the boiling-point isotherm [m]
$\dot{m}(z)$ = the mass-flow rate of water [kg/s] at location z
h_{fg} = the latent heat of vaporization [J/kg]
α = thermal diffusivity [m^2/s]
t = the total time elapsed since the water entered the superheated region (s)
t_z = the time required for the water to penetrate to a distance z.

Equation 4.3.5-11 can be integrated between 0 and z ($0 < z < l$) with the boundary condition $\dot{m}(z=0) = \dot{m}_o$ (defined in Equation 4.3.5-5) to yield the following expression for the mass flow rate of water at location z:

$$\dot{m}(z) = \dot{m}_o - \left(\frac{2}{\pi}\right)^{0.5} \frac{q}{h_{fg}} \frac{z^2}{\left[\alpha w^{-2}(t - t_z)\right]^{0.5}} \text{ for } t_z < t < w^2/\alpha \qquad \text{(Eq. 4.3.5-12)}$$

In this episodic analysis, the total time available for water to penetrate into the superheated zone is limited by the time it takes for the water to drain from the pinch-point aperture (t_d). After this time, the source term for water infiltration, $\dot{m}_o$, goes to zero. Therefore, in Equation 4.3.5-12 the total time elapsed, t, can be approximated as the total drainage time, t_d. In addition, t_z is solved using Equation 4.3.5-9 with $l = z$:

$$t_z = \frac{\pi}{2}\left(\frac{z}{L_3}\right)^4 \frac{w^2}{\alpha} \qquad \text{(Eq. 4.3.5-13)}$$

Equation 4.3.5-12 can then be used to estimate the mass flow rate of water at a particular location in the superheated region during asperity-induced episodic infiltration events. This will be of particular interest in the application discussed below to determine the amount of water that can penetrate a superheated region surrounding a tunnel containing heat-generating waste packages.

4.3.5.5.3 Assumptions

Although the asperity-induced episodic infiltration model provides convenient analytical expressions for the episodicity and water-penetration distances, it also includes a number of important assumptions:

- Although the configuration of the infiltrating weeps is three-dimensional, the flow of water through the fractures is modeled as one-dimensional in the downward direction. Water accumulation and drainage is governed by a weep width that constrains the physical boundaries of accumulation and drainage in the lateral direction.

- All fluid and material properties are modeled as constant over time. In the application presented here, properties were averaged over temperature ranges from ambient (20°C) to boiling (96°C for Yucca Mountain). Distributions were obtained from previous Yucca Mountain reports, as summarized in Table 4.3.5-3.

- Fracture-matrix interaction (e.g., imbibition) is ignored in this analysis. If a significant amount of matrix imbibition exists, the water-penetration distance into the superheated distance will be less.

4.3.5.5.4 Application and Results

The asperity-induced episodic infiltration model is applied to the thermal seepage problem using the input parameters tabulated in Table 4.3.5-3.

Figure 4.3.5-11 shows a cumulative probability plot of the episodicity factor (Equation 4.3.5-8) for two weep widths (0.01 and 1 m) and different flow focusing conditions. The amount of flow focusing depends on weep spacing. Figure 4.3.5-11 shows that the smaller the weep width, the larger the episodicity factor; the episodicity factor is much lower when there is no flow focusing.

Figure 4.3.5-12 shows a plot of the cumulative probabilities for 300 realizations of the water-penetration distance (Equation 4.3.5-9) divided by the superheated distance (Table 4.3.5-3, 9th row) for different widths of the infiltrating water. Approximately 30 percent of the 300 realizations show water penetration to the drift wall when the weep width is equal to 1 m. Only about 15 percent of the realizations show penetration to the drift wall when the weep width was equal to 0.001 m. Figure 4.3.5-12 also shows that the results begin to converge as the weep width approaches a value of 1 m. In the three-dimensional solution presented by Phillips (1996 [DIRS 152005]), a weep width of 1 m yields a solution that is identical to an analogous two-dimensional solution that uses an infinite weep width along the direction of the fracture plane. Therefore, a weep width of 1 m can be viewed as a limiting condition that allows the greatest water-penetration distance for the three-dimensional solution. This value has been used in TSPA calculations of episodicity and flow of water at the drift wall, as described in the next section.

Figure 4.3.5-12 shows a cumulative distribution function of the ratio of the mass flow rates at the drift wall to the initial mass flow rates, $\dot{m}_o$, for 300 realizations with a weep width of 1 m, using Equations 4.3.5-12 and 4.3.5-13. The desired location, z, is set equal to the superheated distance to the drift wall, d. If the time available for infiltration, t (which is set equal to the drainage time, t_d), is less than the time required for the water to reach the drift wall, t_z, then the mass flow rate is set to zero. The majority of the values are near zero because, as shown in Figure 4.3.5-12, the majority of the realizations do not result in water penetration to the drift wall. This distribution can be useful for determining the impact of asperity-induced episodic flow and penetration to the drift wall on performance assessment seepage analyses that evaluate the amount of water that can contact the waste packages.

4.3.5.6 Abstraction for Total System Performance Assessment

The results presented above show that it is very difficult for water flow to reach the emplacement drifts when the drift walls are above the boiling temperature. Under these conditions, seepage into the drifts is greatly reduced and possibly eliminated entirely. The analyses conducted with the mountain-scale coupled-process model (Section 4.3.5.3) and the MSTH model (Section 4.3.5.4) found no seepage into the drift during the thermal period for the HTOM, even with heterogeneity included. The analysis of penetration of episodic pulses through superheated rock (Section 4.3.5.5) showed that it is possible for seepage to occur, but it also found that water did not reach the drift wall under most parameter combinations.

4.3.5.6.1 Reduction of Seepage by the Vaporization Barrier

In the base case TSPA model, the dry superheated zone around the drifts was neglected and seepage was conservatively allowed to occur throughout the thermal period (CRWMS M&O 2000 [DIRS 153246], Section 3.3.3.2.3). This has no effect on the results of the base case nominal scenario because the waste packages and drip shields are still intact during the thermal period, so no radionuclide releases can occur (CRWMS M&O 2000 [DIRS 153246], Section 4.1.2). However, results of other scenarios could be affected (e.g., if there were an unexpected early failure of both drip shield and waste package at the same location).

An extension of the TSPA model to make it more realistic would be to calculate seepage differently (or modify the base case calculation) when the drift wall temperature is above boiling. Seepage could be reduced even when temperatures are subboiling, as they are for the LTOM, but the reduction is more uncertain and more analysis would be required to quantify a sufficient range of conditions to be able to include it in the TSPA model. Another issue, especially for the LTOM, is the effect of forced ventilation. The dryout zone around the drifts caused by removal of moisture by the ventilation system would tend to reduce seepage into the drifts, but that effect is not currently included in the TH or seepage models.

In the following paragraphs, a relatively simple abstraction is described for the reduction in seepage when the drift walls are above boiling (i.e., for the HTOM).

Two types of results are available. The simulations using the mountain-scale coupled-process model and the MSTH model indicate no seepage when the drift wall temperature is above boiling. More extreme conditions were considered using the analytical model of penetration of episodic pulses through superheated rock, and some of those conditions resulted in water reaching the drift. The distribution of reductions in flux calculated with the analytical model is shown in Figure 4.3.5-12. That figure shows that almost three-fourths of the realizations that were modeled resulted in no water reaching the drift. The rest had varying amounts of flow reduction, ranging all the way up to almost no reduction. Average reduction ratio for the 300 realizations is approximately 0.2. The distribution represents a possible range of spatial variation; that is, some locations would be expected to have little reduction in seepage, but most locations would be expected to have seepage reduced to zero, with an average reduction of approximately 80 percent.

The abstraction recommended for TSPA simulations is to sample a random number that varies from 0 to 0.2 and multiply the seepage calculated by the seepage abstraction model by that factor whenever the drift wall is above the boiling temperature. When the drift wall is below boiling, the seepage calculated by the seepage abstraction model should be used without change. This abstraction is easy to implement and covers the range of results given by the TH models. The sensitivity of TSPA results to this random parameter will be an indication of whether the TH seepage reduction is important to the results.

4.3.5.6.2 Effects of Episodicity on Seepage

The mechanism suggested in Section 4.3.5.5 for producing episodic pulses of flow down fractures is not limited to the thermal period, but could occur at any time. It is not clear whether this process actually occurs in Yucca Mountain. It requires that water be trapped in a storage aperture until enough pressure builds up to break through the capillary resistance of a pinch-point aperture. This type of episodic flow has not been observed in Yucca Mountain, and it might not be possible under ambient conditions to trap water for long enough because of possible dissipation by imbibition into the matrix or evaporation. However, because episodic flow pulses could lead to greater seepage into drifts (e.g., CRWMS M&O 2000 [DIRS 153314], Section 6.6.6; CRWMS M&O 2001 [DIRS 154291], Section 6.4.4), it is important to consider the possible impact of this mechanism on TSPA results.

A method for including episodic flow in the seepage abstraction was presented in *Abstraction of Drift Seepage* (CRWMS M&O 2001 [DIRS 154291], Section 6.4.4), though it was not included in the final abstraction because episodic flow was thought to be unlikely. However, that method can now be used to evaluate the effects of asperity-induced episodic flow. In the abstraction method, episodic flow is parameterized by an episodicity factor, which is the fraction of time that flow occurs. Distributions of episodicity factors calculated for asperity-induced episodic flow are presented in Figure 4.3.5-11. As discussed in Section 4.3.5.5.4, the middle curve ($w = 1$ m, $A = a^2$) is considered to be appropriate for use in TSPA simulations. That curve is reasonably well represented as a log-uniform distribution between 10^{-4} and 10^0.

The individual distributions shown in Figure 4.3.5-11 represent spatial variability in the episodicity factor (i.e., they represent a range of episodicity values that could occur at different spatial locations). The three different curves represent uncertainty—the most representative values for the weep width, w, and cross-sectional area, A, are uncertain. The abstraction method (CRWMS M&O 2001 [DIRS 154291], Section 6.4.4) does not allow for spatial variability of the episodicity factor; episodicity effects are represented by a single factor in each TSPA realization. However, the importance of episodicity to TSPA results can be determined by sampling the episodicity factor from an uncertainty range and examining its effect on the results. The log-uniform distribution between 10^{-4} and 10^0 that was suggested above is a reasonable choice for the uncertainty distribution because it encompasses the average values of all three episodicity distributions in Figure 4.3.5-11.

4.3.5.7 Multiple Lines of Evidence

Simulations in the above section show that there is an increase of liquid flux in the condensation zones outside of drying that can account for the phenomenon of water being moved away from the drift and draining in the cooler region of the pillar between two adjacent emplacement drifts. This phenomenon of drainage of water outside an above-boiling region of rock mass is corroborated by observations in the Drift Scale Test being conducted in the ESF. The temperatures in boreholes parallel to the wing heaters in the Drift Scale Test consistently show a heat pipe signature beyond the drying zone of the wing heaters (Birkholzer and Tsang 2000 [DIRS 154608]). The heat pipe signature of a temperature maintained at boiling is an indication of potential water movement in the fractures, as all water collection in the Drift Scale Test has been possible only in those borehole sections when the temperature is at boiling.

In the analysis above, the effect of moisture removal by forced ventilation has not been accounted for. Forced ventilation has the effect of reducing water seeping into the drift. Evaporation of seeped water has been observed in seepage tests being carried out in the ESF and the ECRB Cross Drift. The challenge there is to assess quantitatively the impact on seepage of drying from ventilation.

4.3.5.8 Summary of Uncertainties and Their Treatment

Thermal seepage models, like any other models, are subject to uncertainties due to various factors, such as data, parameters, conceptualization, and numerical model implementation. Of all the uncertainty issues, the ones that contribute the greatest uncertainty to the thermal effects on seepage are different thermal operating modes, the effects of lithophysal cavities on thermal properties, and the heterogeneity of fracture permeability. Studies pertaining to these uncertainty issues are highlighted in the analyses presented above. A more complete list of the uncertainty issues particular to thermal seepage and their treatment is given in Table 4.3.5-4.

4.3.5.9 Summary and Conclusions

Modeling and uncertainty studies have been performed to predict how decay heat from emplaced waste would affect the magnitude and spatial distribution of percolation flux reaching the emplacement drifts, and, in turn, the potential of seepage into the drifts. The effect of TH processes on seepage has been considered for the HTOM and LTOM.

The studies discussed above are based on two separate numerical models (Sections 4.3.5.3 and 4.3.5.4) and an analytical model (Section 4.3.5.5). The results show that it is very difficult for water flow to reach the emplacement drifts when the drift walls are above the boiling temperature. That is, for the higher-temperature repository, the dry superheated zone around the drift possibly eliminates seepage into the drift. The analyses conducted with the mountain-scale coupled-process model (Section 4.3.5.3) and the MSTH model (Section 4.3.5.4) found no seepage into the drift during the thermal period for the HTOM, even with heterogeneity and extreme conditions included. The analysis of penetration of episodic pulses through superheated rock (Section 4.3.5.5) shows that it is possible for seepage to occur, but it also found that water did not reach the drift wall under most parameter combinations.

For the lower-temperature case, the studies in Section 4.3.4.3 show that other than some drying in the fractures below the drift, the decay heat causes little redistribution of moisture or enhancement of fracture liquid fluxes. Therefore, the thermal effect on seepage is insignificant when the temperature is below boiling.

Based on the results of the process models, the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) model during the thermal period has been modified to make it more realistic. The modification was to remove the very conservative assumption of taking the typical percolation flux to be that at 5 m above the drift, and to remove the assumption to neglect the dry superheated zone around the drifts as a vaporization barrier for seepage. However, the recommended extension to the TSPA-SR model still is conservative. Instead of adopting the results of no seepage during the thermal period from the numerical models under expected repository conditions, the TSPA model will use the results of the analytical model of penetration of episodic pulses through superheated rock, where seepage can occur under more extreme conditions than those expected.

4.3.6 Thermal-Hydrologic-Chemical Effects on Seepage and Potential Seepage Chemistry

This section summarizes modeling and uncertainty studies performed for the evaluation of THC effects on seepage and on the chemistry of water and gas in the near-field environment (NFE) that may enter drifts as seepage or through gas flow.

4.3.6.1 Introduction

THC processes may impact seepage through changes in fracture porosity and permeability, fracture unsaturated hydrologic properties (e.g., capillarity), and fracture-matrix interaction. Changes in the chemistry of water that may enter drifts through seepage take place via numerous processes, including water-rock interaction, evaporation or boiling and condensation, interactions with the gas phase, transport processes, and climate changes. Uncertainties in the conceptual models, data used for input and model validation, and predictions of THC effects as they influence seepage and seepage chemistry are discussed in *Drift-Scale Coupled Processes (DST and THC Seepage) Models* (CRWMS M&O 2000 [DIRS 142022]) and its revisions (CRWMS M&O 2001 [DIRS 154426]; BSC 2001 [DIRS 154677]). The TSPA-SR (CRWMS M&O 2000 [DIRS 153246]) was based on an abstraction (CRWMS M&O 2000 [DIRS 123916]) of the data documented in the initial version of *Drift-Scale Coupled Processes (DST and THC Seepage) Models* (CRWMS M&O 2000 [DIRS 142022]). This work is summarized in Section 4.3.6.3. Since the TSPA-SR, several new analyses, models, sensitivity studies, assessments of unquantified uncertainties, and validation studies have been performed; these are documented in the latest revision of *Drift-Scale Coupled Processes (DST and THC Seepage) Models* (BSC 2001 [DIRS 154677]) and in this report (see Sections 4.3.6.4, 4.3.6.5, and 6.1.3.5).

The methods used to evaluate THC effects on seepage and seepage chemistry include the development of conceptual and numerical models, estimation of geochemical parameters such as thermodynamic and kinetic data, model validation using large-scale thermal tests and laboratory experiments, and predictive (process) modeling. This approach was chosen because it provides the means to test the appropriateness of the conceptual model, evaluate uncertainties in different conceptual models, and predict effects on seepage rate and seepage chemistry over time. Uncertainties in some thermodynamic and kinetic parameters were treated using sensitivity studies and comparisons to data from the Drift Scale Test and laboratory experiments. Remaining unquantified uncertainties regarding spatial variability of seepage-relevant formation properties; the distribution of local percolation flux; variability in initial and infiltration water chemistry; and the impact of design decisions regarding ventilation, thermal loading, potential repository area, and drift orientation were addressed through appropriately broadened uncertainty distributions and conservative considerations in the abstraction (CRWMS M&O 2000 [DIRS 123916]). Unquantified conceptual uncertainties were assessed in analogue studies, laboratory experiments, and other corroborating observations.

The conceptual model for THC processes provides a comprehensive basis for modeling the pertinent mineral-water-gas reactions in the host rock under thermal loading conditions as they influence the chemistry of water and gas that may enter drifts during 100,000 yrs. Data are incorporated from the drift-scale calibrated property sets, the UZ flow and transport model, geochemical data (fracture and matrix mineralogy, aqueous geochemistry, and gas chemistry), thermodynamic data (minerals, gases, and aqueous species), data for mineral-water reaction kinetics, and transport data (BSC 2001 [DIRS 154677]). Simulations of THC processes include coupling between heat, water, and vapor flow; aqueous and gaseous species transport; kinetic and equilibrium mineral-water reactions; and feedback of mineral precipitation or dissolution on porosity, permeability, and capillary pressure (hydrologic properties) for a dual-permeability (fracture-matrix) system.

The effect of coupled THC processes on the evolution of flow fields and potential seepage chemistry in the UZ around drifts has been investigated for different potential future climate change scenarios, calibrated property sets, initial mineralogy, and heterogeneous permeability fields.

4.3.6.2 Goal of Drift-Scale Thermal-Hydrologic-Chemical Models

The goals of the models used for prediction of drift-scale THC processes and their abstraction are:

- Provide a conceptual basis and methodology for developing drift-scale THC models
- Validate the THC model by comparing its results to results from field and laboratory experiments
- Identify conceptual uncertainties and address uncertainty through sensitivity studies that vary key parameters
- Predict changes in hydrologic properties resulting from mineral precipitation/dissolution and associated THC effects on flow and seepage
- Predict changes in water and gas chemistry around drifts, which are the potential elements that could enter drifts through seepage or gas flow.

The coupled THC processes important for evaluation of changes in the chemistry of the NFE and effects on flow are illustrated schematically in Figure 4.3.6-1. In particular, the influence of certain UZ hydrologic processes (such as fracture-matrix interaction) and thermal-hydrologic processes (such as the development of a heat pipe) have a strong effect on the chemical evolution of the system.

4.3.6.3 Discussion of Initial Results

The work summarized in this section was performed to support the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]). In addition to providing the basis for the development of the drift-scale THC models, the analyses presented in the initial version of *Drift-Scale Coupled Processes (DST and THC Seepage) Models* (CRWMS M&O 2000 [DIRS 142022]) supply the following:

- Validation of drift-scale THC process model by simulation of the Drift Scale Test and comparison to measured gas and water chemistry collected through August 1999
- Prediction of THC effects around drifts for a higher-temperature backfill design with drift emplacement in the Tptpmn unit (two-dimensional column model at the USW SD-9 borehole)
- Evaluation of different modeled geochemical systems (base case and extended case)
- Evaluation of the effects of changing climate states on THC processes, along with upper- and lower-bound infiltration rates and corresponding drift-scale calibrated property sets.

The base case and extended case geochemical systems were developed to address uncertainties in the geochemical conceptual models and allow for predictions that are less affected by reactions that have larger uncertainties, such as those involving zeolites and clays. The base case geochemical system consisted of calcite, silica polymorphs (i.e., tridymite, cristobalite, quartz, and amorphous silica), gypsum, appropriate aqueous species, and carbon dioxide gas. The extended case system included additional zeolite and clay minerals, ferric iron oxide/hydroxide minerals, and fluorite.

4.3.6.3.1 Validation of the Drift-Scale Thermal-Hydrologic-Chemical Process Model with the Drift Scale Test

Results of the validation analysis showed that modeled carbon dioxide concentrations in the gas phase captured the general trends seen in measured compositions. The base case geochemical system provided a much closer match to measured gas-phase carbon dioxide concentrations and the pH of waters that were collected from boreholes near the boiling zones. Apparent discrepancies between modeled and measured carbon dioxide concentrations were observed for samples collected at boiling temperatures because the sampled gas was mostly steam, with little air, and most of the steam was removed by condensation before analysis. However, when the carbon dioxide concentrations were adjusted for water removed, the trends were qualitatively similar in the boiling intervals (BSC 2001 [DIRS 154677], Section 6.2.7.2). The ranges of modeled and measured pH for waters collected in boreholes near the boiling interval were also shown to be similar. Because the comparisons of the water and gas chemistry from the extended system results were not as good as those from the base case system, the uncertainties associated with model validation were greater for the associated aqueous species (i.e., Al, Fe, K, and pH). These uncertainties are likewise also associated with predictions done with the THC Backfill Seepage Model, described in the following section. However, because the initial water and gas compositions are only known approximately, and their spatial distributions unknown, a quantitative evaluation of the uncertainties associated with the predictions is not feasible. Yet the range of predicted and measured compositions in the drift-scale test for waters that may potentially seep into drifts are not extremely great and the model results generally capture this range.

4.3.6.3.2 Initial Report of Thermal-Hydrologic-Chemical Effects on Flow and Potential Seepage

The effect of coupled THC processes on the time evolution of flow fields in the UZ around drifts was investigated for different climate change scenarios, calibrated property sets, initial mineralogy, and heterogeneous permeability fields. Predictions of the changes in flow around drifts as they could influence seepage were based on simulations of 100,000 yrs, which included a preclosure period of 50 yrs with 70 percent of the heat removed by ventilation. The EDA II design, including backfill (Wilkins and Heath 1999 [DIRS 104247]), was considered as the base case design. This design was used for the TSPA-SR and included a higher-temperature thermal operating mode with 50 yrs of forced ventilation. The predicted extent of the dryout zone and the time of rewetting were different for each modeled climate history and calibrated rock property set, with the upper-bound infiltration showing the smallest dryout zone and earliest time of rewetting of the drift crown. Predicted porosity reductions in the Tptpmn in the NFE were small (less than 1 percent), with minor effects on permeability and thermal-hydrologic processes. The simulation using the upper-bound climate showed the most porosity loss, resulting primarily from continued buildup of calcite (owing to its smaller solubility with increasing temperature) over long time periods. The conclusions drawn from this work, using an initial fracture porosity of 1 percent and homogeneous rock properties within each unit, were that THC processes would have a negligible effect on seepage.

4.3.6.3.3 Initial Report of Thermal-Hydrologic-Chemical Effects on Potential Seepage Water and Gas Chemistry

Predictions of the chemistry of the water and gas that may enter emplacement drifts showed that general trends of carbon dioxide gas and aqueous species concentrations around the drifts did not differ significantly for the different climate states and property sets. Water and gas composition trends predicted around emplacement drifts by the THC seepage models during the early phase of heating and the dryout period were generally similar to trends observed in the Drift Scale Test and predicted with its THC simulations. Rewetting has not yet been observed in the Drift Scale Test, so no field data can be used to evaluate water and gas compositions at the time of rewetting. The THC simulations indicate that concentrations of carbon dioxide gas may increase around the drifts during rewetting (relative to ambient values) and concomitant small reductions in pH may occur.

4.3.6.4 Discussion of Updated Results

The update to *Drift-Scale Coupled Processes (DST and THC Seepage) Models* (BSC 2001 [DIRS 154677]) included several additional models, analyses, validations, and sensitivity analyses that were done after the TSPA-SR. Additional validation of the Drift Scale Test THC model included comparisons to another year of water and gas data, along with evaluation of the effect of different reaction rates and geochemical systems. Some aspects of the THC model data and approach were validated by simulating a plug-flow reactor experiment performed under subboiling (about 94°C) conditions and at an elevated carbon dioxide partial pressure (see Section 4.3.6.7).

Three new drift-scale models were added in the updated report: a no-backfill model in the Tptpmn unit, a Tptpmn model with heterogeneous fracture permeability distributions, and a drift-scale THC model in the Tptpll geologic unit (with no backfill). The update also incorporated better-constrained thermodynamic and kinetic data, an improved consideration of initial mineral precipitation, increased reactive surface areas in fractures, and a stronger coupling of permeability to porosity changes. The base case geochemical system was modified to include fluorite, and the extended case system was changed with the addition of opal-ct and the removal of sepiolite and potassium-smectite. Numerous sensitivity studies were performed, including:

- Different in-drift designs (backfill versus no-backfill)
- Potential repository host rock units (Tptpmn versus Tptpll)
- Alternative conceptual models of pertinent geochemical systems (base case versus extended case)
- Effects of uncertainty in thermodynamic data (free energies and activity coefficient models)

- Treatment of certain mineral-water reactions for specific minerals (kinetic rate constants, reactive surface areas, and equilibrium versus kinetic conceptual models)

- Fracture permeability-porosity relations during mineral precipitation/dissolution

- Stochastic realizations of strong initial spatial heterogeneity in fracture permeability with accompanying effects on THC processes around drifts.

4.3.6.4.1 Thermal-Hydrologic-Chemical Model Validation

The model was validated by comparing measured gas and water chemistry from the Drift Scale Test to the results of simulations using the Drift Scale Test THC model. In particular, simulation results were compared to measured gas-phase carbon dioxide concentrations and the chemistry of waters collected from hydrology boreholes during the test. Comparisons of model results to measured changes in carbon dioxide concentrations over nearly three years (Figure 4.3.6-2) show that the model captures the initial rise in concentration in all of the borehole intervals where comparisons were made, areas that have very different thermal histories.

Figure 4.3.6-3 shows variations in pH, calcium, and chloride for two borehole intervals from the Drift Scale Test between the initial measured matrix pore water composition and the simulated concentrations for the base case and extended case geochemical systems, as well as for additional sensitivity studies on selected geochemical models and parameters. Comparisons between observed and modeled water chemistry (pH, chloride, sulfate, and calcium) and carbon dioxide concentrations in the gas phase from the Drift Scale Test indicate that a limited set (base case) of aqueous species, minerals (calcite, silica phases, gypsum), and gases (water, air, and carbon dioxide) can describe the general evolution of Drift Scale Test waters with respect to pH, carbon dioxide, and conservative anions. A more complete geochemical system (extended case), including a wide range of aluminosilicates (such as feldspars, clays and zeolites), yields modeled aqueous silica concentrations closer to those observed, as well as providing information on the concentrations of additional species (potassium, aluminum, iron, and fluorine). The initial extended geochemical system shifted the pH to values higher than those observed and to correspondingly lower gas-phase carbon dioxide concentrations. After the initial model results were documented, revision of less well-constrained thermodynamic data for smectites and zeolites, reduction in the reaction rate of anorthite, and minor changes in the mineral assemblage in the extended case geochemical system resulted in simulated compositions that were more consistent with measured water and gas compositions from the Drift Scale Test. However, gas phase carbon dioxide concentrations and pH still compare to measured values somewhat better with the base case geochemical system.

The lower chloride concentrations in the water samples collected from boreholes, compared to the initial pore water (Figures 4.3.6-3e and 4.3.6-3f), indicate that these waters have experienced little interaction with the matrix pore water. The modeled matrix pore water, however, shows a decrease in the concentration of chloride of about 15 percent as a result of the imbibition of dilute condensate draining through fractures. The minimal fracture-matrix interaction under thermal-hydrologic conditions supports the basic model of a limited area for liquid imbibition resulting from low liquid saturations in fractures and the equations embedded in the modified AFM (BSC 2001 [DIRS 154677]).

Model validation was also performed through simulations of the plug-flow reactor laboratory experiment (Kneafsey et al. 2001 [DIRS 154460]; BSC 2001 [DIRS 154677], Section 6.7). These results are discussed in Section 4.3.6.7.

4.3.6.4.2 Thermal-Hydrologic-Chemical Effects on Flow and Potential Seepage

Simulations of a no-backfill design predict a smaller dryout zone (particularly below the drift) and a somewhat earlier time of rewetting than simulations of a design that includes backfill. This is primarily the result of a slightly lower thermal load imposed in the simulations performed for the updated report, although the removal of backfill caused the crown to become somewhat hotter and the base cooler. In all simulations, the dryout zone continued to expand until about 600 yrs, when a wetter climate with a greater infiltration flux was imposed. Depending on the modeled scenario, the maximum extent of the dryout zone is predicted to be between 6 and 10 m above the drift center, and the predicted time of rewetting at the drift crown varies between 800 and 1,200 yrs.

The predicted reduction in porosity in the NFE over 100,000 yrs for the Tptpmn THC no-backfill model (homogeneous permeability) is less than 3 percent of the initial fracture porosity, which reduces the permeability by less than one order of magnitude. This is somewhat greater than the reduction predicted for the Tptpmn THC backfill model (a less than 1 percent change in fracture porosity), but it is still relatively minor. The permeability calculation is based on uniform areas of precipitation in plane parallel fractures; the actual effects on permeability and flow in heterogeneous fractures with rough surfaces and nonuniform mineral precipitation could be greater. Comparison of the purely thermal-hydrologic simulation results 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 after rewetting of the drift wall results almost entirely from precipitation of calcite and amorphous silica. Amorphous silica contributes to most of the initial mineral precipitation up until the early rewetting stage, with maximum deposition spreading above the drift in a zone roughly coincident with the maximum extent of the dryout zone (8 to 10 m from the drift center). The silica dissolves slowly after rewetting. Calcite precipitates throughout the boiling and later cooling stages, becoming most of the mineral precipitated at 100,000 yrs.

Heterogeneity in fracture permeability can have varied effects on thermal-hydrologic processes, including flow focusing and irregularity in isotherms and liquid saturation. TH and THC simulations were performed for three heterogeneous fracture permeability realizations (with a range in permeability of four orders of magnitude) under the mean infiltration rate climate change scenario (6 mm/yr to 600 yrs, 16 mm/yr to 2,000 yrs, and 25 mm/yr to 100,000 yrs) for the Tptpmn unit (DTN: LL000114004242.090 [DIRS 142884]). The range in permeability is consistent with that used in the ambient seepage analyses discussed in Section 4.3.1. Although some regions at the outer edge of the dryout zone have high fracture saturation, the water does not reach the drift wall when the dryout zone is well developed (Figure 4.3.6-4). Areas of highest initial liquid saturation also having lower permeability and generally located above the drift tend to show the greatest reduction in fracture permeability, down to about 25 percent of the initial value after 20,000 yrs in some regions (Figure 4.3.6-5). This localized permeability reduction tends to cause some additional flow focusing, but the changes are considerably less than the initial range in permeability. The corresponding maximum fracture porosity reductions are approximately 5 percent of the initial value, resulting in permeability reductions of less than one order of magnitude (about 75 percent). Porosity reductions for the extended geochemical system were slightly greater than those for the base case system, as a result of additional minerals precipitating and somewhat higher silica concentrations in the extended case simulated waters. The maximum amount of amorphous silica precipitated was 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 (and low-permeability) zones near the drift.

4.3.6.4.3 Thermal-Hydrologic-Chemical Effects on Potential Seepage Water and Gas Chemistry

THC simulations in the *Drift-Scale Coupled Processes (DST and THC Seepage) Models* report (BSC 2001 [DIRS 154677]) predicted notable differences in pH and carbon dioxide concentrations, depending on the geochemical system considered (base case or extended case). This resulted in large part from the dissolution of anorthite (one component in a plagioclase feldspar solid-solution phase) to form clays and zeolites, which occurred under ambient conditions and increased under thermal loading. Thermodynamic and kinetic data were revised for the updated report so that the initial water composition was closer to a steady-state composition under ambient conditions, resulting in better-constrained water compositions, pH, and carbon dioxide concentrations predicted under thermal loading. This significantly reduced the differences between predictions using the base case and extended case geochemical systems. In general, pH values were lower and carbon dioxide concentrations higher in the base case than in the extended case. The extended case geochemical system may overestimate the effect of mineral-water reactions on the geochemistry of waters and gases, and may therefore provide an upper limit on the extent of changes in chemical and hydrologic properties around emplacement drifts. In both cases, fairly dilute and near-neutral to moderately alkaline water compositions are predicted around drifts, with pH values in the range of 7 to 9 and gas phase carbon dioxide concentrations generally below 10,000 ppmv. As the last water evaporates, what remains behind becomes highly concentrated but nearly immobile (Figure 4.3.6-6). Calculated water and gas compositional trends in the Tptpmn and Tptpll units were similar because the models share the same mineralogy and water chemistry.

Spatial variations in water chemistry around the drift were not strongly affected by permeability heterogeneities. The highest concentrations of conservative species were in the low-permeability, high-liquid saturation areas that underwent boiling at the base of the heat pipe zone. Variations in pH and chloride around the drift for the heterogeneous and initially homogeneous Tptpmn THC models during the peak dryout time of 600 yrs are shown in Figures 4.3.6-6 and 4.3.6-7. Areas of higher pH developed at the base of the boiling zone (i.e., the edge of the dryout zone, shown as white in the figures), primarily because of carbon dioxide loss, but also as a result of hydrolysis reactions in the extended case. Percolation of water from the surface eventually pushes this higher-pH water below the drift (the model domain actually extends to the surface and to the water table). The areas of higher pH are generally below and to the side of the dryout zone in the extended case simulations, whereas in the base case the higher pH waters are in a narrower region mostly above and to the side because this is the area of greatest carbon dioxide depletion. Chloride concentrations show the large increases expected in the boiling zone and the dilution effect in the condensation zone. Strong fracture drainage of the more dilute condensate water results in a well-developed plume extending over 100 m below the drift.

An uncertainty that was not considered was the effect of lithophysal porosity on THC processes. Obvious effects of lithophysae would be to provide a larger volume for the vapor phase and to force a greater flux of water into the matrix and fractures if the lithophysae act as capillary barriers. This could result in changes in gas-phase carbon dioxide transport and increased fracture-matrix interaction. Increased fracture-matrix interaction and condensation in lithophysal cavities (and subsequent drainage into connected fractures) could result in less-dilute seepage water chemistry and increased mineral precipitation in fractures.

4.3.6.5 Model Development Since the Issuance of the Updated Report

Recent model development has involved studies of coupled processes for an expanded range of temperatures. This work was based on the EDA II repository design (Wilkins and Heath 1999 [DIRS 104247]), which specified an initial thermal load of 72.7 kW/acre (1.45 kW/m in the drift) and a ventilation period of 50 yrs, during which 70 percent of the decay heat would be removed. The thermal load of the EDA II design gives rise to above-boiling temperatures in the rocks near the emplacement drifts for hundreds of years. Model development conducted since the update of *Drift-Scale Coupled Processes (DST and THC Seepage) Models* (BSC 2001 [DIRS 154677]) has focused on lower-temperature options in which the rock temperature does not exceed the boiling point of water anywhere in the potential repository. The LTOM considered a linear thermal load of 1.13 kW/m and removal of 80 percent of decay heat by ventilation for 300 yrs. The two operating modes, the HTOM and the LTOM, are referred to as the higher-temperature case and the lower-temperature case, respectively.

Several simulations were performed for the lower-temperature case and for uncertainty analyses on the higher-temperature case. These sensitivity simulations included different top boundary (i.e., soil zone) gas phase carbon dioxide concentrations and different initial and boundary water compositions (pore water and perched water). Different initial and infiltrating water chemistry have a greater effect on the chemistry of potential seepage than the changes in boundary carbon dioxide concentrations. The major difference in the simulations for the lower-temperature case is the absence of a dryout zone. Because of evaporation, the waters tend to have relatively high concentrations of conservative anions (e.g., chloride) at a given liquid saturation, but the fracture liquid saturations are near the residual saturation of one percent, well below what would cause seepage. Details regarding the effects on potential seepage chemistry are provided in Section 6.3.1.5. The effects of THC processes on porosity and permeability in the LTOM were slight (less than 1 percent over 20,000 yrs) because amorphous silica, the primary phase that results in porosity loss during boiling, is generally undersaturated except in areas adjacent to the drift wall where substantial evaporation has taken place.

4.3.6.6 Abstraction for Total System Performance Assessment

Abstraction of drift-scale THC processes is described in Section 6.3.1.6. This includes the composition and fluxes of potential seepage water at specific locations at the drift wall and the associated gas phase compositions.

4.3.6.7 Multiple Lines of Evidence

The emplacement of heat-generating nuclear waste in a potential geologic repository at Yucca Mountain will result in enhanced water-rock interaction around the emplacement drifts compared to the rates of reaction occurring under ambient conditions. As the waste package heats the surrounding environment, water present in the matrix and fractures of the nearby rock may vaporize and migrate through fractures to cooler regions where condensation would occur. The condensate would dissolve gases and minerals, and mineralized water flowing under gravity back towards the heat source would evaporate, depositing the dissolved minerals. Such mineral deposition would reduce porosity and permeability above the potential repository, thus altering the flow paths of percolating water (Nitao and Glassley 1999 [DIRS 154486]). Natural analogue studies of water-rock interaction in geothermal systems and along igneous contacts, as well as hydrothermal field and laboratory experiments, provide multiple lines of evidence for THC effects on permeability and porosity that would change seepage (Apps 1995 [DIRS 154615]). A number of natural analogue examples and field and laboratory studies are summarized below, followed by a more detailed examination of the Yellowstone geothermal system and a tuff dissolution-precipitation experiment. The processes demonstrated by these examples are then related to Yucca Mountain, with an emphasis on how differences in scale could influence the impact that these processes may have on the performance of the potential repository.

4.3.6.7.1 Effects of Water-Rock Interaction on Fluid Flow: Natural Analogues

The effects of water-rock interaction on important hydrogeological properties, such as permeability and porosity, have been widely documented for a number of geologic settings. Geothermal systems and igneous contacts, such as those discussed below, illustrate how heat and water can cause mineral dissolution and precipitation, resulting in changes in formational fluid flow properties. Water-rock interaction tends to be more extensive in long-lived, water-saturated geothermal systems than along shallow intrusive and extrusive contacts occurring above the water table, where short-lived thermal perturbations provoke minimal mineralogic changes. These geologic systems encompass the time scales and heterogeneities necessary to evaluate models for the potential Yucca Mountain repository and provide important information needed to build, calibrate, and evaluate numerical models for the Yucca Mountain system. Three geothermal systems and three magmatic contact areas are summarized in the following paragraphs.

Imperial Valley Geothermal Fields, California–The effects of water-rock interaction have been studied at a number of geothermal fields (Salton Sea, East Mesa, Heber, Brawley, Cerro Prieto, and the Dunes) within the Imperial Valley (e.g., Schiffman et al. 1985 [DIRS 154644]; Cho et al. 1988 [DIRS 154599]). Elders (1987 [DIRS 154632]) examined the Salton Sea geothermal field as a potential natural analogue for evaluating processes related to radioactive waste storage. Low-permeability carbonate-cemented sandstones form the primary caprock, and represent the first of four distinct hydrothermal alteration zones. Fractures provide fluid flow pathways that cut across low-permeability shale interbeds. Complex sequences of fracture mineralization observed at the Salton Sea indicate that fractures episodically opened and sealed throughout the life of the geothermal system (Elders 1982 [DIRS 154602]). Silica sealing has been documented at the Dunes geothermal system (Bird and Elders 1976 [DIRS 154601]). Seven distinct zones of sandstones and conglomerates located in what originally were the most permeable strata within the sedimentary section underwent intensive silicification, resulting in a significant reduction in porosity and permeability. The formation of these silicified zones was interpreted to be due to the lateral migration of hot brine to a cooler environment.

Wairakei Geothermal Field, New Zealand–The Wairakei geothermal field illustrates the influence of fractures and alteration on fluid flow. Grindley (1965 [DIRS 154663]) noted that wells intersecting normal faults have high permeabilities, whereas nonproductive wells usually intersect hydrothermally cemented rocks with intrinsically low (less than 1 millidarcy) permeabilities. Bruton (1995 [DIRS 100105]) observed that vein mineral assemblages typically contain fewer phases than those found associated with the matrix and interpreted that fracture, vein, and vug minerals are the products of a fluid-dominated system, whereas the more complex matrix alteration mineralogy results from high rock-water ratios. The intensely altered, impermeable rocks overlying the main reservoir at Wairakei serve to protect the producing zone from cold water encroachment.

Medicine Lake Geothermal System, California–The Quaternary Medicine Lake volcano in northern California is host to a higher-temperature geothermal system. Exploratory drilling has revealed that the geothermal reservoir is capped by hydrothermally-altered rock that is rich in smectite-group swelling clays that form a barrier to fluid flow (Hulen and Lutz 1999 [DIRS 154600]). Glassy dacitic to rhyolitic tuffs and pumiceous lavas have been strongly altered to smectitic clays, calcite, zeolites, quartz, potassium feldspar, hematite, and pyrite. This argillic alteration mineral assemblage forms a hydrologic barrier between a shallow, cool groundwater zone and a deeper, hot geothermal reservoir.

Banco Bonito Obsidian Flow, New Mexico–The effects of elevated temperatures on tuff mineralogy can be examined along the contact between the Banco Bonito obsidian flow and the Battleship Rock Tuff, located on the southwest rim of the Valles Caldera in northern New Mexico (Stockman et al. 1994 [DIRS 117820]). Upon eruption, the Banco Bonito flow (with an estimated eruptive temperature of 850°C) came into contact against the porous tuff, resulting in some baking and deformation of the immediate tuff contact zone. Stockman et al. (1994 [DIRS 117820]) conducted detailed geochemical transects in the tuff outward from the obsidian contact but observed relatively small changes in chemical composition and only minor hydrothermal alteration, and suggested that the studied contact area was located above the local water table, resulting in little water-rock interaction.

Paiute Ridge Intrusive Complex, Nevada–The Paiute Ridge intrusive complex (Matyskiela 1997 [DIRS 100058]; Lichtner et al. 1999 [DIRS 121006]), located about 40 km northeast of the potential repository, consists of a series of dikes and domed lopoliths emplaced between the Paintbrush and Timber Mountain tuffs, above the local water table. Thermal modeling of the intrusions suggest that they are large enough (at least 30 m) to have sustained boiling around the intrusive margins for thousands of years. Lichtner et al. (1999 [DIRS 121006]) noted several physical changes in the tuffaceous host rock resulting from the intrusions, including the presence of a gray to black vitrophyre within 0.5 to 1 m of the contact, with abundant anastamosing joints that are parallel to the contact. The degree of contact welding decreases within 1 to 3 m from the contact, and devitrification and partial alteration of volcanic glass to clay extends from the outer margin of the vitrophyre up to 15 m from the contact.

Determining the nature and intensity of the alteration of the tuff caused by intrusive activity is complicated by variable amounts of hydrothermal alteration of the tuff host rock that occurred prior to intrusion of the basaltic dikes and sills. Matyskiela (1997 [DIRS 100058]) studied the Papoose Lake basalt sill in the Paiute Ridge complex and suggested that all tuffs within 50 m of the sill contact have been altered to some extent. Matyskiela observed that the most intense alteration was focused along the margins of widespread (1 to 15 m) near-vertical fractures that parallel extensional faults in the area. The tuff matrix glass and pores within 1 cm of the fractures have been completely replaced by an impermeable and nonporous zone of clinoptilolite and cristobalite, and later-formed chalcedony and rare calcite fill most fractures. Matyskiela interpreted that the reduced matrix permeability and the sealing of fracture margins caused by this alteration event would result in enhanced fluid flow through the fractures. Lichtner et al. (1999 [DIRS 121006]) question several of these interpretations, such as whether alteration is most intense closest to the intrusive contact and the fracture margin mineralization is related to the Paiute Ridge intrusive event.

Grants Ridge Intrusion, New Mexico–The Grants Ridge intrusion consists of a shallow basaltic plug that intruded into nonwelded, pumice-rich rhyolitic tuff and volcaniclastic sediments (WoldeGabriel et al. 1999 [DIRS 110071]). A 10-m wide aureole developed around the 150-m wide plug, characterized by partial melting, changes in color, brecciation, and stoping. Despite initial temperatures greater than 1,000°C at the contact zone, only minor devitrification of the surrounding tuff was observed. WoldeGabriel et al. (1999 [DIRS 110071]) interpreted the lack of hydrothermal alteration in the contact zone to indicate that the plug was intruded into an unsaturated environment.

4.3.6.7.2 Effects of Water-Rock Interaction on Fluid Flow: Observations from Field and Laboratory Experiments

Field and laboratory experiments provide important information regarding water-rock interaction under controlled conditions. Many of these experiments have been used to address issues of permeability reduction and self-sealing in geothermal fields and enhanced oil-recovery operations. Key factors influencing mineral dissolution and precipitation include fluid chemistry, rock mineralogy, ratio of reactive surface area to solution mass, reaction temperature, and occurrence of condensation and boiling processes. Two of the main mechanisms for silica sealing are cooling of silica-saturated waters and boiling. Operators of geothermal fields often experience silica scaling problems with geothermal brines as they are flashed and cool (Mroczek 1994 [DIRS 154621]). The precipitation of silica polymorphs (such as amorphous silica) is enhanced when fluids that are supersaturated with respect to silica flow slowly through rocks with large surface areas (Wells and Ghiorso 1991 [DIRS 154645]). Boiling can result in even greater amounts of silica precipitation because all dissolved silica will be precipitated as a fluid boils to dryness. The following section summarizes a series of experiments that describe the effects of water-rock interaction on permeability and porosity for a number of rock types. While the experiments encompass a range of temperatures (50° to 250°C) similar to those predicted for the potential Yucca Mountain repository, one important difference is that most of the experiments were conducted under saturated conditions, which would tend to promote increased water-rock interaction. In spite of this difference, the experimental results can still be used to constrain and validate coupled process THC models for the Yucca Mountain system.

Permeability Changes in Hydrothermal Flow-Through Experiments–A series of experiments were performed to observe silica dissolution and precipitation in intact granite and Yucca Mountain ash-flow tuff samples (Morrow et al. 1981 [DIRS 142169]; Moore et al. 1983 [DIRS 154631]; Moore et al. 1986 [DIRS 142166]; Moore et al. 1994 [DIRS 154630]; Daily et al. 1987 [DIRS 131816]). In these experiments, water was flowed through rock samples with an applied temperature gradient and changes in rock permeability and fluid chemistry were monitored. For the granite, permeability decreased one to two orders of magnitude over the 1- to 3-week duration of the experimental run. Changes in effluent fluid chemistry indicated initial silica supersaturation, which declined with time until reaching quartz solubility concentrations after about 6 days. Scanning electron microscopy and petrographic analyses showed regions with precipitated fibrous silica and patchy masses of silica, quartz, and calcium-rich zeolites within the granite. In one experiment, almost all the cracks near the cooler edge were filled with silica, whereas half the cracks near the heated side were open. The large change in permeability relative to the small amount of mineralization suggests that the precipitates formed "bridges" that clogged cracks, having a great effect on permeability.

In contrast to the granite experiments, little change in permeability was observed for the flow-through experiments conducted by Moore et al. (1986 [DIRS 142166]) involving Topopah Spring and Bullfrog ash-flow tuff samples over the time and spatial scale of the experiments. The much smaller reduction in permeability was attributed to the tuffs having much higher porosities and larger aperture flow paths that would be less easily clogged by mineralization. Changes in water chemistry over time suggest that the rate of silica dissolution in the tuff was significantly greater than silica reprecipitation. While the temperatures of these experiments ranged from 90° to 250°C, with higher temperature conditions resulting in increased dissolved silica concentrations, elevated pore pressures of 1 to 10 mPa indicate that boiling did not occur, in part accounting for the minimal amounts of mineralization. Daily et al. (1987 [DIRS 131816]) flowed water through a reopened healed natural fracture in Topopah Spring welded tuff and observed significant permeability reduction for flow through the fracture occurring at temperatures greater than 89°C.

Chigira and Watanabe (1992 [DIRS 154641]) also investigated the effect of hydrothermal reactions on fracture permeability. In their experiments, water saturated with silica was injected into polished granite fracture segments with apertures ranging from 0.05 to 0.1 mm. Negative temperature gradients (from hot to cold) of 50° and 100°C/m were employed for the two runs. In one experiment, system permeability decreased by more than four orders of magnitude because of fracture plugging. Scanning electron microscopy and optical microscopic observation of the fracture surfaces indicate that amorphous silica particles precipitated evenly over the various mineral phases of the granite, with increased mineralization occurring along the cooler fracture segments.

An experimental investigation of silica self-sealing incorporating boiling was performed by Rimstidt et al. (1989 [DIRS 142190]). A heat pipe reactor containing chips of ash-flow tuff from Yucca Mountain was operated for 30 days. Within the experimental apparatus, three distinct zones were observed. In the condensation zone, etching and dissolution features evidenced dissolution of the tuff. In the center zone, few indications of dissolution or precipitation were observed. In the bottom region, extensive precipitation of amorphous silica, iron oxyhydroxides, stilbite, and possibly clays was observed, resulting in a tightly cemented region along the face of the heater. Such mineralization would lead to significant permeability reductions.

Evidence of Water-Rock Interaction from Enhanced Oil Recovery Operations–Water-rock interaction has been evaluated in a variety of diagenetic studies associated with thermal recovery of heavy oils. Field studies have used two approaches to document water-rock interaction associated with steam flooding: looking at changes in pre- and post-flood rock mineralogy and monitoring changes in produced fluid chemistry. Laboratory experiments have examined both fluid and rock chemistry to identify the primary reactions controlling water-rock interaction occurring in sandstone reservoirs under steam-flood conditions.

A detailed study of heavy oil-bearing lithic-rich sandstone was conducted on core samples collected from the Clearwater Formation at the Cold Lake Oil Sands pilot site in eastern Alberta (Sedimentology Research Group 1981 [DIRS 154634]; Hutcheon 1984 [DIRS 154633]). High pH steam was continuously injected into the field for two years. Temperatures reached 230° to 260°C in the stratigraphic section of interest during the course of the steam flood.

The steamed core was more indurated than the pre-steam core, with increases in smectite and corresponding decreases in kaolinite and porosity within and immediately below the steam flood interval. The effective porosity and permeability of the altered sandstones were reduced by post-steam smectite grains, which formed thick rims on framework crystals. Kaolinite replacement by smectite resulted in a volume increase, also serving to reduce porosity and permeability.

Steam flooding of the Aberfeldy heavy oil field (Saskatchewan) resulted in only minor mineralogic changes, consisting of the formation of small amounts of illite and chlorite (Lefebvre and Hutcheon 1986 [DIRS 154637]). The absence of authigenic smectite in the post-steam flood core samples likely results from the lack of sodium-bearing minerals in the quartzose sandstones. This study demonstrates the importance of lithology in determining which secondary minerals will form as a result of water-rock interactions.

In another study that shows the importance of mineralogy in water-rock interaction, Hutcheon and Abercrombie (1990 [DIRS 154638]) monitored the composition of produced waters from three thermal recovery oil wells at Tucker Lake, Alberta. Steam was injected in each well for up to 90 days, followed by 7 months of pumping. Reservoir temperatures during the post-steam injection production phase ranged from 95° to 186°C, with temperatures progressively decreasing over time. Early recovered waters were dilute as a result of condensed steam. However, as production proceeded, fluid compositions became more saline as formation waters mixed with the condensate. While sodium and chloride contents for all produced waters increased with time, potassium contents stabilized after 50 days of production, suggesting that its concentration was controlled by mineral reactions. Geochemical modeling of produced fluids (Hutcheon and Abercrombie 1990 [DIRS 154638]) suggests that the activity of potassium is controlled by reactions involving potassium-feldspar and illite, while the $Ca^{2+}/(H^{+})^{2}$ activity ratio is controlled by the calcite-carbon dioxide reaction.

Autoclave and flow-through laboratory experiments using natural and synthetic oil field sands document the formation of significant quantities of smectite in the pore spaces, resulting in permeability decreases. Experiments conducted by Boon (1978 [DIRS 154643]) using Athabasca shales show that considerable quantities of montmorillonite formed as a result of water-rock reactions. Experiments conducted using Cold Lake oil sands (Boon et al. 1983 [DIRS 154640]) resulted in the formation of analcime, chlorite, smectite, and calcite at the expense of quartz, kaolinite, and dolomite. In a similar series of experiments, Kirk et al. (1987 [DIRS 154639]) also observed decreases in kaolinite and dolomite, increases in smectite and calcite, and a pronounced decrease in the overall permeability (50 percent to 98 percent overall reduction) of the steam-flood cores. Similar decreases in permeability (65 percent to 78 percent reduction), primarily caused by the formation of smectite (iron-saponite), were observed in a series of coreflood experiments conducted by Zhou et al. (1999 [DIRS 154635]).

Boon (1978 [DIRS 154643]) observed that silica-rich solutions were produced by heating deionized water together with oil sands, and that the amount (and rate) of silica dissolution is positively correlated with temperature and pH. The change in dissolved silica concentrations correlates with temperature, and the measured concentrations obtained from a number of experiments lie between those predicted by the quartz and chalcedony geothermometers (Gunter et al. 1992 [DIRS 154642]). This dissolution process is analogous to the condensation end of a heat pipe, where the dilute fluid would rapidly dissolve silica. The condensate could either flow into cooler rock, becoming supersaturated with respect to silica, or flow back into the boiling zone, where the silica concentration of the solution would increase as boiling progresses. Both scenarios would lead to silica precipitation and reduced permeability for certain portions of the formation.

4.3.6.7.3 Self-Sealing at the Yellowstone Geothermal System

Mineral dissolution and precipitation and associated changes in permeability resulting from water-rock interaction have been observed in a number of geothermal systems (Grindley and Browne 1976 [DIRS 154531]; Fournier 1983 [DIRS 154614]). One of the best examples of self-sealing has been documented at the Yellowstone geothermal system through detailed studies of continuously cored research boreholes (White et al. 1975 [DIRS 154530]; Keith et al. 1978 [DIRS 106316]; Keith and Muffler 1978 [DIRS 152663]). Water-rock interaction at Yellowstone has resulted in extensive hydrothermal alteration, especially along veins and fractures, where most fluid flow occurs. Matrix permeability measurements, lithologic and alteration descriptions, and fracture and vein characterization were conducted on core samples from two of these boreholes (Y-5 and Y-8) to evaluate the effects of lithology and hydrothermal alteration on permeability and porosity (Dobson et al. 2001 [DIRS 154547]; Dobson et al. 2001 [DIRS 154503]). Hydrothermal self-sealing appears to have generated the existing permeability barrier that delineates the top of the convecting geothermal system at Yellowstone. Changes in pressure and temperature in the Y-8 borehole associated with the transition between conductive and convective flow correspond to a zone of silicification with large porosity and permeability reductions. The presence of bladed calcite near this interval and elevated delta oxygen-18 values of hydrothermal quartz suggest that the silica seal may have formed in response to transient boiling events associated with depressurization (Sturchio et al. 1990 [DIRS 154524]).

While the Yellowstone system and the potential Yucca Mountain repository share many of the same THC processes, the effects of the processes are expected to differ significantly because of large differences in scale between the two systems. The Yellowstone geothermal system is a liquid-dominated, convecting geothermal system with much higher fluxes of heat and fluid than those predicted for the Yucca Mountain system. The dissolution, transport, and precipitation of silica are highly dependent on system temperature, mineralogy, and fluid flux rate, as well as whether boiling occurs. Rates of silica dissolution and equilibrium silica concentrations in geothermal fluids at Yellowstone are significantly higher than those predicted for Yucca Mountain because of the higher temperatures (170° to 240°C) encountered in the Yellowstone system (White et al. 1975 [DIRS 154530]). Downhole water samples from the Y-7 and Y-8 wells have silica concentrations of 364 and 290 mg/L, respectively (Sturchio et al. 1989 [DIRS 154529], p. 11028), more than three times greater than those predicted for the Yucca Mountain system (Kneafsey et al. 2001 [DIRS 154460]) and twice that observed in the waters collected from higher-temperature intervals in the Drift Scale Test (BSC 2001 [DIRS 154677], Figure 24). The outflow of silica-enriched waters from geysers and hot springs at Yellowstone resulted in the formation of extensive silica sinter deposits. While rates for fluid flow within the Yellowstone system are difficult to quantify, Sturchio et al. (1987 [DIRS 154525], p. 12029) estimate a conservative formational velocity of 1,500 m/yr (4.8×10^{-5} m/s) at Yellowstone, about four to five orders of magnitude higher than those predicted for Yucca Mountain. Even higher rates would be expected for focused flow along fractures. It is also difficult to accurately estimate the rate of silica precipitation and concomitant permeability reduction for the Yellowstone system. Most of the wells drilled at Yellowstone from 1967 to 1968 experienced significant plugging or complete sealing by 1992 (Fournier et al. 1993 [DIRS 154527], p. 33), suggesting that silica sealing accompanying boiling occurs fairly rapidly. All these factors have to be scaled properly before using the Yellowstone example to semi-quantitatively validate the Yucca Mountain THC simulations.

4.3.6.7.4 Tuff Dissolution and Precipitation in a Boiling, Unsaturated Fracture: Laboratory Experiments and Numerical Simulations

As part of an ongoing effort to evaluate multiple lines of evidence for THC effects on flow in fractured media, a laboratory experiment (Kneafsey et al. 2001 [DIRS 154460]) and related numerical simulations (BSC 2001 [DIRS 154677], Section 6.7; Bodvarsson 2001 [DIRS 154669], Attachment 4, pp. 7 to 38; Dobson 2001 [DIRS 154922]) were performed to investigate plugging of fractures caused by mineral dissolution and precipitation. The laboratory experiment consisted of two stages: dissolution of crushed Topopah Spring ash-flow tuff in a plug-flow apparatus and mineralization resulting from fluid flow and boiling within a vertical fracture. For the accompanying simulations, TOUGHREACT V2.2 and V2.3 was used to model the tuff dissolution and precipitation processes. The experiment and simulations can be used to evaluate the processes and time scales of tuff dissolution and secondary mineral precipitation, and serve to validate use of the TOUGHREACT codes. The experiment and simulations indicate that boiling and concomitant mineralization could cause significant reductions in fracture porosity and permeability on a local scale.

Experiment Description and Results–A two-part experiment was conducted to evaluate tuff dissolution and fracture sealing (Kneafsey et al. 2001 [DIRS 154460]). To replicate mineral dissolution by condensate water in fractured tuff (Figure 4.3.6-8), deionized water equilibrated with 50,200 ppm carbon dioxide was flowed for 1,500 hours through crushed Yucca Mountain Tuff (75 to 150 micron size) at 94°C and a rate of 25 ml/hr (DTN: LB0011THCDISSX.001 [DIRS 153380]). The reacted water exiting the tuff column was collected and regularly sampled for major dissolved species, total alkalinity, electrical conductivity, and pH. The resulting steady-state fluid composition (achieved after 230 hours) had a total dissolved solids content of about 140 mg/L; silica was the dominant dissolved constituent.

A portion of the steady-state reacted water was flowed at 10.8 ml/hr into a 31.7-cm tall, 16.2-cm wide vertically oriented planar (saw-cut) fracture in welded Topopah Spring Tuff that was maintained at 80°C at the top and 130°C at the bottom (DTN: LB0101THCPRCPX.001 [DIRS 154577]). The two blocks were separated with 17.7-micron gold shims; however, the hydraulic aperture calculated using the initial air permeability was about 31 microns. The dimensions of the fracture, the magnitude of the temperature gradient, and the flow rate were based on the relations derived by Phillips (1994 [DIRS 154459]; Phillips 1996 [DIRS 152005]). The fracture began to seal within five days, as indicated by a declining outflow rate and leaks in the inlet side of the fracture. Increased pressure was required to maintain the flow of water at 10.8 ml/hr following the leak sealing. After several unsuccessful attempts to plug leaks and the near-zero rate of effluent collection, it was concluded that the aperture was effectively sealed.

The fracture was opened at the conclusion of the experiment to examine the precipitate location, mineralogy, and morphology (Figure 4.3.6-9). Aperture sealing to fluid flow occurred with only 3 to 20 percent of the total fracture volume filled with solid precipitate, primarily composed of amorphous silica (Kneafsey et al. 2001 [DIRS 154460]). The precipitate was deposited almost exclusively at fracture locations where adjacent matrix temperatures exceeded the boiling point. The precipitate morphology appeared to vary as a function of temperature. Porous, veiny, honeycomb-like bridging structures formed in the hottest regions (about 120°C), similar to morphologies noted for Single Heater Test samples (CRWMS M&O 1999 [DIRS 129261], pp. 6-40 to 6-43). Wall-coating precipitate with vitric luster and bridging structures was deposited at locations that had temperatures near 110°C. Solid, well-formed bridging structures with minor amounts of wall coating occurred at locations that had temperatures near 100°C, and fine-grained precipitate was observed in a few locations in the subboiling region.

4.3.6.7.4.1 Simulation Description and Results

Numerical simulation of the laboratory experiment was conducted using TOUGHREACT V2.3 in two different phases: tuff dissolution and fracture sealing. The descriptions and results of these simulations are described in this section.

Tuff Dissolution Plug-Flow Simulations–A series of isothermal TOUGHREACT V2.3 simulations were performed to model tuff dissolution using a 149-element one-dimensional mesh with dimensions and interface areas identical to those of the plug-flow experiment, plus one additional boundary element to obtain the appropriate outlet conditions (BSC 2001 [DIRS 154677], Section 6.7). Initial mineralogy used for plug-flow simulations was obtained from the Tptpmn (tsw34) matrix composition. An initial fluid composition was calculated using SOLVEQ/CHILLER V1.0 and the measured pH and carbon dioxide concentration of the experimental inlet water. Trace amounts of other dissolved constituents were used in the simulation to reduce computational problems caused by zero values. The plug-flow column was liquid-saturated with no separate gas phase present. The flow rate (25 ml/hr) and temperature (94°C) of the dissolution simulation were set to the values used in the experiment.

Simulation runs were conducted using TOUGHREACT V2.2 and V2.3. Most of the TOUGHREACT V2.3 concentration profiles have steady-state compositions that are slightly higher than the corresponding values obtained from the TOUGHREACT V2.2 runs because the change in water density was incorporated into the mineral surface area calculations in the new version of the code.

Two grain-size models were tested to evaluate the sensitivity of surface area values on kinetic mineral reactions. The first model employed mineral surface areas calculated using spherical grains with a diameter of 60 μm, with clay minerals represented by rectangular plates with dimensions $60 \times 60 \times 1.2$ μm. The second model used spherical grains with diameters of 120 μm and clay minerals with dimensions $120 \times 120 \times 2.4$ μm. Large (up to 100 percent) differences observed for sodium, silica, and calcium concentrations between simulations using the two models result from the twofold difference in calculated initial surface areas (DTN: LB0011THCDISSM.002 [DIRS 154578]).

The calculated concentrations of sodium and silica for the 60-μm grain size (i.e., larger surface area per unit volume) plug-flow simulations closely match the fluid compositions observed in the experimental study (BSC 2001 [DIRS 154677], Section 6.7). The predicted concentrations for the major (greater than 1 mg/L) dissolved species (with the exception of bicarbonate) are within a factor of two of the measured average steady-state concentrations. Differences between the modeled and measured values in pH and alkalinity result from cooling and degassing of the experimental samples after exiting the tuff dissolution column. The outflow compositions match the simulated results closely after they have been corrected for these processes using SOLVEQ/CHILLER V1.0.

Fracture Plugging Simulations–A series of two-dimensional simulations were performed to model fracture sealing using a variety of mesh designs, each with dimensions identical to those in the tuff fracture experiment. The injected fluid composition was taken from measured values obtained from the experiment, and the rock mineralogy was considered to be similar to that used for the plug-flow experiment. The initial fracture permeability was set to the observed experimental conditions, while the flow rate and fracture width were reduced by half (5.4 ml/hr and 15.5 μm, respectively) to account for the half-symmetry model used. To simplify the simulation, the rock matrix blocks were assigned a zero permeability to force the injected water to flow through and interact only with the fracture elements. Amorphous silica was allowed to precipitate under equilibrium conditions to remove uncertainties associated with kinetically controlled nucleation and growth. Because the formation of colloidal silica results in an extremely high surface area, making kinetic precipitation of silica extremely rapid at boiling, equilibrium precipitation conditions are a reasonable proxy for the fracture plugging simulation.

Two mesh designs were employed to resolve the sharp chemical and liquid saturation gradients present in the fracture. Both designs contain two columns of rock blocks and one column of fracture blocks. The outermost rock column consists of elements with fixed temperatures to approximate the experimental temperature gradient (80° to 130°C). One of the mesh designs has 317 elements per column, each 1 mm in height. The other is a variably discretized mesh, with 177 elements per column that range in height from 0.25 to 5 mm; the finer gridding is present in the transition area between vapor-phase and two-phase conditions. Maximum time steps for the simulations are restricted by the minimum gridblock size, with maximum times of

0.3333 seconds for the 1-mm spacing and 0.0833 seconds for the variable spacing. Fluid is injected in the uppermost fracture element, and the lowermost fracture element is assigned a very large volume (greater than 10^{50} m^3) to act as a constant pressure boundary.

The initial results of these simulations indicate the generation of a nearly isothermal region, with an overlying water column above and a vapor zone below (Figure 4.3.6-10). The precipitation of amorphous silica at the base of the two-phase zone accounts for all of the porosity (and thus permeability) reduction in the fracture system. The zone of mineralization (Figure 4.3.6-10) appears to be more restricted in vertical extent in the simulations than was observed in the fracture-sealing experiment (Figure 4.3.6-9). A gradual buildup in pressure occurs in the top of the fracture system with time, resulting in a corresponding downward shift of the base of the boiling zone. Silica precipitation for a given fracture element near the base of the boiling zone results in local porosity reductions of about 60 percent. Additional precipitation in a given element block is retarded by the downward shift in the boiling front resulting from the increase in pressure, which in turn results from the throttling of the fracture (Figure 4.3.6-11). Silica precipitation and porosity reduction continue to follow the boiling front downward, spreading the effects of boiling and concomitant mineralization. Some of the differences between the experiment and the simulations may result from variability in the two-dimensional fracture surface, as well as from fluctuations resulting from fluid leaks and a short-term power outage that occurred during the experiment.

The experiment has a steep temperature gradient, resulting in a narrow boiling zone. Although the grid resolution was as low as 0.25 mm, the transition to dryout was too sharp to obtain full mass conservation given the current implementation in TOUGHREACT V2.3. Therefore, the rate of sealing is underestimated in the simulations by about 25 percent. Significant permeability reduction occurred within 1 to 10 days after the initiation of fluid flow for both the experiment and the simulations.

4.3.6.7.4.2 Applicability to Yucca Mountain Processes: Scaling Effects

It is important to consider differences in scale between the laboratory experiment and associated simulations, along with predicted conditions for the potential Yucca Mountain repository. A number of factors (e.g., thermal gradient, fluid flux, fracture aperture) serve to enhance the amount of silica dissolution, transport, and precipitation and the corresponding fracture permeability reduction in the experiment described above. Table 4.3.6-1 gives a comparison of these factors.

One key issue to address is the rate of potential fracture sealing for the Yucca Mountain system. Fracture sealing occurred rapidly (about 5 days) in the laboratory experiment. A number of factors must be considered in evaluating these data and scaling them to the NFE:

- Water flow rate in fractures (reflux of water via heat pipe effect)
- Fracture apertures and geometry
- Thermal gradient and thickness of boiling front and condensation zone
- Mobility of boiling front with time
- Fracture-matrix interaction
- Effective mineral surface area in condensation zone.

The fracture aperture used for the tuff experiment falls within the range observed at Yucca Mountain, so the key differences between the Yucca Mountain system and the experiment are fracture flow rates (fluid flux) and the width of the boiling zone (gradient). The ratios of fluid flux rates to thermal gradients in the experiment and the potential Yucca Mountain system can be used for approximate scaling calculations to predict how long it would take to plug fractures at the potential repository (Bodvarsson 2001 [DIRS 154669], Attachment 4, pp. 37 to 38). If the width of the boiling front over which silica precipitation occurs can be scaled approximately by the thermal gradient, then the rate of fracture sealing (plugging) can be estimated as:

$$Plugging_{YM} = (Plugging_{EXP}) \times (\frac{FluidFlux_{EXP}}{FluidFlux_{YM}}) \times (\frac{Gradient_{EXP}}{Gradient_{YM}}) \qquad \text{(Eq. 4.3.6-1)}$$

Where YM indicates Yucca Mountain and EXP indicates the experiment. For Yucca Mountain plugging, this is 5 days $\times$ 20,000 $\times$ 210, or approximately 60,000 yrs. This estimated rate of fracture sealing is slower than the rate obtained by Nitao and Glassley (1999 [DIRS 154486]), whose THC simulations for the potential Yucca Mountain repository predict that a porosity reduction of greater than 90 percent for the area 6 m above the drifts will occur 1,500 to 4,000 yrs after waste emplacement if boiling conditions last that long. In comparison, the current higher-temperature design drops below boiling at the drift wall approximately 1,200 yrs after waste emplacement.

The processes controlling the rate of fracture plugging are more complex than this simple scaling calculation suggests. The mineralogy, effective mineral surface area, and temperature control the amount of silica that can dissolve in the condensate. The rate of downward fluid flow from the condensation zone to the boiling zone serves as the limiting factor to the amount of silica transport and resulting mineralization that can occur in the fractures. As noted above, the rate of fracture fluid flux at Yucca Mountain is predicted to be about 20,000 times lower than the rate used for the laboratory experiment. Water flow at Yucca Mountain is controlled by several factors, such as surface infiltration rates (which vary on regional and climatic scales), focused flow along high permeability faults and fractures, and reflux of fluids associated with condensation above the drift zones. Localized zones with elevated flux rates within the boiling front would be most susceptible to silica self-sealing. The geometry and apertures of fractures are important aspects of fracture sealing. As the results of the experiment and simulations indicate, small amounts of total porosity reduction (via mineralization) are required along sharp, stationary boiling fronts and within narrow apertures to seal a fluid conduit. As individual pathways seal, water will flow into larger aperture regions where there is less capillary control buffering the flow. During the evolution of sealing, this may cause fluids in later-generation flow paths to flow faster.

4.3.6.7.5 Summary of Multiple Lines of Evidence for Thermal-Hydrologic-Chemical Processes

The effects of water-rock interaction on permeability and porosity can be observed in geothermal systems and along igneous contacts, as well as in hydrothermal experiments. Liquid-dominated geothermal systems, such as Wairakei and Yellowstone, exhibit extensive hydrothermal alteration resulting from water-rock interaction at elevated temperatures. Parameters such as fluid chemistry, initial rock mineralogy and permeability, the degree of fracturing, fluid flux, and the duration and intensity of heating all influence the degree and nature of mineral dissolution and precipitation that takes place over time. Much less extensive changes are observed along igneous contacts in the UZ (e.g., at Banco Bonito and Paiute Ridge), where the amount of fluid available for water-rock interaction is greatly reduced and the thermal perturbation tends to be much shorter in duration. Field and laboratory experiments confirm these general observations and highlight the importance of processes such as boiling and condensation in controlling mineral precipitation and dissolution. When applying the results of these experiments and associated models to the Yucca Mountain system, proper scaling of the magnitude of THC processes must be applied to assess the potential impact of these processes on potential repository system performance.

4.3.6.8 Summary of Uncertainties and their Treatment

The uncertainties associated with the results of simulations in *Drift-Scale Coupled Processes (DST and THC Seepage) Models* (BSC 2001 [DIRS 154677]) were considered acceptable given the intended purpose of the model, the results of validation studies, and the use of the results by other models (e.g., the TSPA-SR [CRWMS M&O 2000 (DIRS 153246)]). To further reduce the uncertainty in the predictions of THC effects on flow around drifts, seepage, and seepage chemistry, the following sources of uncertainty should be examined in a more systematic fashion:

- Uncertainties in the effective mineral-water reactive surface areas in heterogeneous unsaturated fractured rock (this issue is being addressed through continuing and new laboratory studies, the planned ECRB Cross Drift thermal test, and sensitivity studies)
- Uncertainties in thermodynamic data
- Uncertainties in kinetic data
- Uncertainties in geochemical conceptual models (e.g., mineral solid solutions and precipitating mineral assemblages)
- Uncertainties in fracture hydrologic parameters (i.e., fracture porosity and unsaturated hydrologic properties)
- Uncertainties in thermal-hydrologic conceptual models (e.g., vapor-pressure lowering, enhanced vapor diffusion) and their effects on THC processes
- Uncertainties introduced by code implementations and numerical errors (e.g., grid-induced errors such as orientation and refinement).

Key conceptual and parametric uncertainties regarding the prediction of THC processes related to seepage and their validation by thermal testing and laboratory experiments are summarized in Table 4.3.6-2. Other issues that specifically relate to uncertainties in the geochemical aspects of the THC models, and to predicting the water and gas composition directly at the drift wall, are listed in Table 6.3.1.8-1.

4.3.6.9 Summary and Conclusions

The treatment of coupled THC processes in the UZ is an analysis of a natural barrier that is an important item for waste isolation (YMP 2000 [DIRS 149733]). The work summarized in this section contributes to the analyses and modeling data used to support performance assessment. The analysis of coupled THC processes in the UZ does not directly support any of the principal factors of the postclosure safety case addressed in the repository safety strategy (CRWMS M&O 2001 [DIRS 154951], Volume II, Section 4.1). However, the other factor for site recommendation consideration, effects of heat on flow, is addressed by the analysis of coupled THC processes, which simulate the effect of mineral dissolution and precipitation on the permeability of the fracture continuum.

The effects of THC processes on seepage and on the chemistry of potential seepage water and gas have been evaluated through drift-scale THC model simulations for a range of operating temperatures and designs (see Section 4.3.6.5), validation using the ongoing Drift Scale Test (see Section 4.3.6.3.1), and laboratory experiments (see Section 4.3.6.7.2). The results of these simulations and analyses, which are based on a limited range of input parameters, indicate that mineral precipitation will not affect flow around the drifts to a degree greater than that already produced by the natural variability in hydrologic properties. Simulations have reproduced the results of a laboratory experiment showing fracture sealing within several days. With appropriate time and spatial scaling of percolation fluxes and thermal gradients, the results are consistent with long-term models that predict relatively small changes in fracture permeability. Predictions of ranges in water and gas compositions, also based on a limited set of input parameters, indicate a fairly restricted range in the chemistry of potential seepage water. In zones where the fracture liquid saturation is above the residual saturation of one percent, the waters are fairly dilute and neutral to mildly alkaline (i.e., pH in the range of about 7 to 9). Model validation with the waters collected from near-boiling to below-boiling zones in the Drift Scale Test have captured the overall trends in water chemistry of reactive and nonreactive solute species and pH. Changes in pH are strongly linked to changes in gas-phase carbon dioxide concentrations, the trends of which have also been reproduced by model simulations of the Drift Scale Test.

Many uncertainties associated with the prediction of coupled THC processes as they affect seepage are difficult to assess or have not yet been addressed systematically. The more important issues have been summarized and their status briefly assessed. THC model validation encompasses many of the uncertainty issues and has generally been successful with experiments of short duration for which the initial conditions are known. Uncertainties arising out of ranges in parameters that have not been assessed could be further reduced through additional field thermal testing, laboratory experiments, and modeling.

4.3.7 Thermal-Hydrologic-Mechanical Effects on Seepage

4.3.7.1 Introduction

Section 4.3.7 summarizes the modeling and uncertainty studies performed to determine the effects of coupled THM processes on seepage of liquid water into emplacement drifts. Sections 4.3.1 through 4.3.4 discuss how, at ambient preemplacement conditions, the emplacement drift acts as a capillary barrier to divert water around the drift opening so seepage fluxes will be lower than percolation fluxes. Analysis of seepage under ambient conditions puts emphasis on factors that determine whether water reaching the drift wall will, in fact, seep into the drift. This section focuses on how the THM coupled processes change the near-field permeability and affect the magnitude and spatial distribution of the percolation flux in the vicinity of the drift. These, in turn, affect seepage threshold and seepage potential.

Like all such models, THM seepage models are subject to uncertainties resulting from conceptualization, parameters, and data. In particular, the degree of complexity in THM coupling incorporated into the numerical model to assess its impact on seepage represents a significant uncertainty. Until now, no transient fully three-way coupled THM computer simulator was available to study the potential Yucca Mountain site. For the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]), two-way coupled TH, TM, and hydromechanical processes have been calculated separately or in a sequential snapshot approach. In this approach, TH responses are calculated first, followed by a separate TM analysis to calculate thermal stresses, which is used in a third analysis to calculate fracture permeability changes. In most of these analyses, the rock mass is treated as a continuum (implicitly modeling fractures), while a few attempts have been made to model the rock mass with discretely defined fractures. Since the TSPA-SR, the two-way coupled analysis with discretely defined fractures has been revised and extended. In addition, a new numerical model for transient, fully coupled THM continuum analysis of a fractured media has been developed and applied. Since the TSPA-SR, this model has been used to assess uncertainties in a transient, fully coupled analysis where the significance of THM processes on the percolation flux are examined.

A further uncertainty is associated with what property parameters are assigned for the mechanically induced permeability changes in the fractured rock. Such parameters may include fracture normal stiffness and residual fracture apertures. These need to be tested or calibrated against field measurements at an appropriate scale.

A number of these uncertainties are addressed in the following sections. Modeling studies discussed include the use of alternative modeling approaches and consideration of two different thermal operating modes for below-boiling and above-boiling temperatures within the rock mass.

4.3.7.2 Goal of Thermal-Hydrologic-Mechanical Models for Seepage

These studies are intended to provide insight into how drift excavation and the decay heat from emplaced waste would affect near-field rock permeability and the magnitude and spatial distribution of percolation flux around a potential emplacement drift (and, consequently, the potential of seepage into the drifts) for two different thermal operating modes. Two alternative conceptual and numerical models will be used: the distinct-element model and the fully coupled THM continua model.

4.3.7.3 Distinct Element Analysis

4.3.7.3.1 Discussion of Initial Results

In support of the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]), a calculation to provide an estimate of TM effects on fracture permeability was conducted, as documented in *Calculation of*

Permeability Change Due to Coupled Thermal-Hydrological-Mechanical Effects (CRWMS M&O 2000 [DIRS 149040]). The method used in this calculation was to simulate the TM behavior of a region of fractured rock that surrounds a section of a long horizontal emplacement drift in the Topopah Spring Tuff at Yucca Mountain. The stress field in the rock mass surrounding emplacement drifts in a potential repository at Yucca Mountain will be altered by excavation of drifts and by the heating and cooling cycle associated with emplacement of radioactive waste. The directions and magnitudes of the principal stresses will change significantly as a result of thermal loading, then will revert during cooldown. Compressive stress will build up rapidly in the host rock, especially after the end of the forced ventilation period. The stress field will gradually decay as the temperature in the rock decreases.

Rock mass permeability is an important TH property for assessment of potential drift seepage. The potential repository host rock is a fractured, densely welded ash-flow tuff. Because the rock has low matrix permeability, the rock mass permeability can be conceptualized as mainly associated with fractures, and fracture permeability is highly dependent on fracture deformation. These fractures will deform as stress conditions evolve. Two types of fracture deformation will contribute to THM coupling: normal displacement perpendicular to the fracture plane and shear displacement parallel to a fracture plane. It is widely accepted that the hydrologic behavior of a fractured rock mass is controlled by a relatively few well-connected fractures. Thus, a model that incorporates discrete fractures was used. Fracture deformation during various phases of the heating-cooling cycle is used to predict changes in rock mass permeability.

The rock mass surrounding an emplacement drift was simulated in three dimensions as a rectangular prism 50 m wide, 60 m high, and 30 m thick. A cylindrical (5.5-m diameter) horizontal drift was excavated through the region. The simulated region was intersected by three sets of fractures: one vertical set oriented parallel to the drift, one vertical set oriented perpendicular to the drift, and one horizontal fracture set. Two fracture densities were used for each set of fractures: a low fracture density (0.1/m) for regions more than 15 m from the drift and a high fracture density (0.5/m) for regions within 15 m of the drift. These fracture densities are lower than those observed in situ and used in TH modeling (CRWMS M&O 2000 [DIRS 151964]). However, the lower fracture density is appropriate because not all fractures are geomechanically active (i.e., free to deform or slide) or hydrologically conductive. The fracture densities calculated by Albin et al. (1997 [DIRS 101367], Drawings OA-46-296, OA-46-297, OA-46-298, OA-46-299) for the Tptmn include a large number of sealed and partially sealed fractures that are expected to have relatively little effect on mechanical and hydrologic properties. Descriptive fracture statistics provided by Albin et al. (1997 [DIRS 101367], p. 82) suggest that approximately four out of five fractures contain at least some secondary mineral in-filling. In sections of the ESF main drift, mapping studies also included fractures with trace lengths as short as 30 cm (Albin et al. 1997 [DIRS 101367], p. 10). The shorter fractures are expected to have a relatively small impact on mechanical and hydrologic properties.

Moreover, in practice, a trade-off exists between fracture density and the permissible volume of the inner (fractured) model, given the available memory resources and the computational requirements of the numerical code used for the calculations. Use of a higher fracture density would have mandated a smaller inner model given available computational resources.

Stresses equivalent to the in situ stresses were imposed on the sides and top of the prism. Since this calculation was primarily concerned with fracture deformation, the stress boundary conditions were chosen for the vertical sides of the model to provide a lower limit on normal stress across vertical fractures, thus making it easier for them to open and/or slip. This boundary condition is most appropriate for the regions near the edge of a repository. The base of the prism was fixed in the vertical direction, but allowed to move in the horizontal directions. Fracture deformation values estimated at a series of times were then used to compute permeability change in a cross section perpendicular to the emplacement drift. These values for permeability change were then contoured for different times.

The methodology for estimating TM effects on permeability incorporated a distinct element model that can capture the mechanical behavior of discrete fractures. In the distinct-element method, the rock mass is composed of an assembly of deformable blocks that are interfaced by discontinuities. Fractures in the rock mass are entered individually into a distinct-element code (3DEC V2.0), and both normal and shear deformation are predicted for the individual fractures. The example calculation discussed in this section uses fracture spacings appropriate for the middle nonlithophysal region of the repository.

The thermal field imposed by the emplacement of nuclear waste containers was simulated within the 3DEC V2.0 distinct element code using a conduction-only thermal model that calculates temperatures, thermally induced stresses, and displacements in a half-space. The thermal model is weakly coupled to the discrete element mechanical simulator in 3DEC V2.0, in that thermal stresses and displacements were incorporated into the predicted stress and displacement fields. The thermal load of the model was based on the EDA II design (Wilkins and Heath 1999 [DIRS 104247]), in which ventilation is used to remove heat from the emplacement drift for the first 50 yrs after emplacement. The EDA II design shows a "spike" in the pillar temperature starting at 50 yrs, when ventilation ceases, followed by a cooling between 50 and 100 yrs. A simple step function was used for the thermal power input. Power was supplied at a constant level of 460 watts for 50 yrs to simulate the ventilation phase, then raised to 615 watts and held constant for 100 yrs, then reduced. Overall, at locations more than a few meters away from the drift, the temperatures matched those predicted using by TH models well enough for use in this calculation. This heating schedule produced temperatures similar to the maximum pillar temperature but over a longer time, followed by a rapid cooldown.

The numerical model was then used to estimate stress and deformation values in the block at a series of times after emplacement. Normal and shear deformation were predicted for multiple locations on each fracture face. The results included two-dimensional images of permeability multipliers calculated from predicted values of normal and shear displacement of fractures, and indicate that the major TM effect on fracture permeability occurs during cooldown for both shear and normal deformation.

Results indicate that shear deformation of fractures during the cooldown of a potential geological repository may cause the fracture permeability in a region within two drift diameters of a drift wall to increase by as much as an order of magnitude. Specifically, shear deformation on vertical fractures during cooldown produces the maximum amount of permeability change, and increases in permeability of a factor of five may occur on vertical fractures at distances beyond two drift diameters from the drift wall.

Results also indicate that normal deformation of fractures may cause permeability to increase as well, but to a lesser extent than shear deformation. Normal deformation during heating may cause permeability to decrease significantly within one drift diameter of the drift wall. During cooling, vertical fractures above the drift may open and the permeability can increase by a factor of two.

4.3.7.3.2 Updated Model Developments

The distinct-element analysis has been revised and extended to provide a more robust estimate of the TM effects on fracture permeability in the rock mass around an emplacement drift. This work is new since the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]), and is documented in Blair (2001 [DIRS 155005]). In the new analyses, the higher-temperature and lower-temperature cases were simulated. The higher-temperature case simulates a heat input of 1.45 kW/m of drift applied with a forced ventilation period of 50 yrs, during which 70 percent of the decay heat is removed. Details of this input scenario and updated thermal parameters are discussed in Section 4.3.5. In addition, fixed displacement boundary conditions were used on the sides of the model. This analysis also used the cubic law to relate changes in fracture aperture to changes in rock mass permeability. The analysis incorporated the effect of shear slip along fractures by computing both stress reduction and fracture dilation as a function of shear displacement. Three fracture sets were used, including two subvertical sets and one subhorizontal set that were mapped in the middle nonlithophysal unit of the Topopah Spring Tuff. An emplacement drift orientation of 72° was used. Temperatures used in the simulations were predicted using the NUFT V3.0s code and the line-averaged-heat-source, drift-scale, thermal-hydrologic (LDTH) model L4L4 (CRWMS M&O 2000 [DIRS 151825]), which is appropriate for determining the evolving stress and deformation fields in the TM model. The use of L4C4 is consistent with process models used in TSPA features, events, and processes and is expected to bound the thermal driving forces for the TM model. This LDTH model is one of 31 LDTH submodels used in the TH process-level model that generates repository-wide thermodynamic conditions for the TSPA-SR. The L4C4 LDTH model is located just east of the center of the repository (Easting 170501 m, Northing 233807 m). This model is two-dimensional; the emplacement drift is located in the tsw35 hydrologic unit. Because this is a two-dimensional model, no heat loss from repository edge effects is included. This ensures that the highest temperatures and the greatest thermal gradients drive TM processes in the simulation.

Input parameters used for the simulations were derived primarily from *TBV-332/TBD-325 Resolution Analysis: Geotechnical Rock Properties* (CRWMS M&O 1999 [DIRS 126475]), and are listed in Table 4.3.7-1.

Permeability changes were determined at eight time increments: 10, 50, 55, 100, 200, 400, 1,000, and 100,000 yrs after waste emplacement. Data developed for the higher-temperature case have been entered into the Technical Data Management System (DTN: LL010109723123.011 [DIRS 154664]). The data were developed using EARTHVISION V5.1 and 3DEC V2.0.

The model inputs for the LTOM analyses were identical to the high temperature case, except that temperatures from the LTOM thermal-hydrology analyses were used.

4.3.7.3.3 Results from Updated Distinct Element Analysis

Results from this analysis indicate that the principal stress direction will rotate from primarily vertical to primarily horizontal, oriented perpendicular to the emplacement drift axes as temperatures in the rock near the emplacement drifts increase. Compressive stresses as high as 60 MPa are predicted in narrow zones in the floor and roof of the drift. The rotation of the principal stress direction is due primarily to the boundary condition imposed at the center of the pillars. In this analysis, the rock at pillar center was not allowed to move in the horizontal direction perpendicular to the drift. This caused horizontal compressive stress to increase as the rock tried to expand during heating. This analysis also indicates that fracture permeability further into the rock will be substantially reduced for vertical and subvertical fracture sets, while the permeability of horizontal fracture sets will remain relatively unchanged.

The changes in predicted fracture permeability field develop soon after the end of the forced ventilation period in association with temperature increases in the near-field rock at that time and persist throughout the 1,000-yr simulation interval. Figure 4.3.7-1 shows the distribution of calculated permeability ratios at 55 yrs, and Figures 4.3.7-2 to 4.3.7-4 show histograms of the calculated permeability ratios in different fracture sets at 55, 1,000 and 100,000 yrs. Figure 4.3.7-1 shows fracture permeability in the first 2 m of rock forming the emplacement drift wall increasing substantially. Fracture permeability may also increase in the region above the drift, extending to one drift diameter above the drift crown. However, increases in permeability greater than one order of magnitude are not predicted beyond 0.5 m from the drift except in the region above the drift and away from the drift wall; a substantial decrease in permeability is predicted throughout the rock mass.

Figures 4.3.7-2 and 4.3.7-3 show that at 55 and 1,000 yrs, permeability may be substantially reduced for vertical and subvertical fractures, while the permeability of horizontal fractures remains relatively unchanged. This change in the predicted fracture permeability field develops soon after the end of the ventilation period (in association with a temperature increase at that time) and persists throughout the 1,000-yr simulation interval.

Upon cooldown, fracture permeability may increase above initial values for horizontal and vertical fractures. Figure 4.3.7-4 shows that the increase in fracture permeability upon cooldown is in the range of one to two orders of magnitude.

The permeability ratio distributions for horizontal and vertical fracture sets are summarized in Tables 4.3.7-2 and 4.3.7-3, respectively. The results for the two vertical fracture sets, which are very similar, have been combined and the bins representing decreased permeability ratio broadened to encompass two orders of magnitude. The results show that permeability ratios for the majority of the horizontal fractures at all times predicted in this study have remained about the same, to within one order of magnitude. The permeability ratios for most vertical fractures decreased by several orders of magnitude during the period between 50 and 1,000 yrs. At 100,000 yrs, the permeability ratio for both horizontal and vertical shows values well in excess of one, indicating that these fractures reopen upon cooling.

This recent analysis predicted higher stresses and larger changes in fracture permeability than were predicted in the calculation presented in Section 4.3.7.3.1. These changes are due to the use of a different set of boundary conditions and a revised relationship between fracture deformation and permeability change.

The THM distinct-element model has also been used to simulate rock mass behavior and estimate changes in fracture permeability for the LTOM case. This case is designed to keep the drift wall temperature well below boiling throughout the lifetime of the repository. The inputs for the LTOM predictions were identical to those for the HTOM case, with the exception that LTOM temperatures were used. Results for the LTOM case show that, as expected, the stress levels in the rock mass are lower than for the HTOM case and that the highest stresses occur after the end of ventilation at 300 yrs after emplacement. In addition, the results show that the fracture permeability remains basically unchanged for the first 300 yrs of storage while ventilation is maintained. A typical histogram of permeability ratio values for times during ventilation period (Figure 4.3.7-4a) shows results for 100 yrs after emplacement.

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 yrs after emplacement (Figure 4.3.7-4b), and gradually changes over time, with fracture permeability decreasing by 3 orders of magnitude in approximately 20 percent of the vertical fractures by 1,000 yrs 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 smaller in magnitude, and affect fewer fractures, than the changes in fracture permeability predicted for the HTOM case. The HTOM case predicted a decrease of 6 orders of magnitude in permeability for most vertical fractures during the period from 55 yrs to more than 1,000 yrs after emplacement.

The following conclusions concerning the pre-cooldown period result from the distinct element analysis:

- The primary effect of the TM processes will be to rotate the principal stress direction from primarily vertical to primarily horizontal, oriented perpendicular to the emplacement drift axes. Compressive stresses as high as 60 MPa are predicted in narrow zones in the floor and roof of the drift.

- Permeability will be substantially reduced for vertical and subvertical, while the permeability of horizontal fracture sets will remain relatively unchanged.

- The change in the predicted fracture permeability field develops soon after the end of the ventilation period (in association with a temperature increase at that time) and persists throughout the 1,000-yr simulation interval.

- Heating associated with waste emplacement is predicted to cause the drift walls to displace inward as horizontal stress levels increase. This movement will cause fracture permeability to increase substantially in the first two meters of rock around the emplacement drift. Fracture permeability may also increase in the region above the drift, extending to one drift diameter above the drift crown. Increases in permeability greater than one order of magnitude are not predicted beyond 0.5 m from the drift, except in the region above the drift.

4.3.7.3.4 Model Validation for Distinct Element Model

The distinct-element model has been used to simulate deformation observed in the Drift Scale Test conducted in the middle nonlithophysal unit. Deformation measurements using multiple-point borehole extensometer systems have been made in several boreholes in the Drift Scale Test. Moreover, deformation measurements were made in three boreholes during excavation of the heated drift section of the Drift Scale Test drifts.

The distinct-element model was used to simulate deformation in several of the boreholes during excavation of the drift and the first 545 days of heating of the Drift Scale Test. Rock property inputs used for these simulations were the same as those used for the emplacement drift simulations discussed above and listed in Table 4.3.7-1 and temperatures were taken from TH simulations of the Drift Scale Test presented in the *Thermal Tests Thermal-Hydrological Analyses/Model Report* (CRWMS M&O 2000 [DIRS 151964]).

Results of the validation show that the overall response of the distinct element model correctly predicts both the magnitude and trends of the deformation observed in the Drift Scale Test. Details of the validation are presented in Blair (2001 [DIRS 155005]).

4.3.7.4 Coupled Thermal-Hydrologic-Mechanical Continua Model

One of the major advances since the initial work presented in *Calculation of Permeability Change Due to Coupled Thermal-Hydrological-Mechanical Effects* (CRWMS M&O 2000 [DIRS 149040]) is the implementation of a coupled THM continua code and its application to the study of drift-scale THM effects on flow and seepage. This work consisted of a distinct element analysis used to calculate permeability changes caused by mechanical and TM responses. The new coupled continuum model provides an opportunity to study THM effects using an alternative conceptual and numerical model. In addition to changes in permeability, changes in percolation flux can be directly assessed.

4.3.7.4.1 Description of a Fully Coupled Thermal-Hydrologic-Mechanical Continua Model

Since the initial work, and in parallel with the continued TM analysis using the distinct-element method, a fully coupled THM code has been implemented. It is a joining together of two well-established codes through carefully designed linkage routines. The first is the TOUGH2 V1.5 code, which uses the dual-permeability continuum (fracture and matrix continua) approach. It has been proven successful in predicting the temperature and moisture distribution of field experiments at Yucca Mountain, including the Single Heater Test (CRWMS M&O 1999 [DIRS 129261]) and the Drift Scale Test (CRWMS M&O 2000 [DIRS 151964]). The second is the industry-standard FLAC3D V2.0 code, which can calculate fracture rock and soil mechanical processes in a continuum model.

The general conceptual model for THM processes may be described as a multiphase, non-isothermal, and deformable medium where voids of the rock skeleton are filled partially with liquid water and partially with gas. Thus, it is a three-phase system (gas, liquid, and solid) in which each of the fluid phases has two components (water and air). The gas phase is modeled as an ideal gas mixture composed of dry air and water vapor; the liquid phase consists of water and dissolved air. The mechanical behavior of the porous and fractured media responses to changes in temperature, skeletal effective stress, and strain, with accompanying porosity and permeability changes. Coexisting fluid and solid components are modeled as in local thermal equilibrium (i.e., locally they are at the same temperature). While a few main fractures may be discretely defined within a rock matrix, the main part of the fractured and porous rock is treated as a single continuum or multicontinuum (fracture system and matrix blocks). In a multicontinuum model, the temperature and pressure may be different in the matrix and fractures, while the total stress (as opposed to the effective stress) is modeled as the same in both continua. Four types of conservation equations are needed to fully describe such a system, including two mass balance equations for the two fluid components, one energy balance equation, and one momentum conservation equation of rock deformation forces.

The fluid mass balance equation of a coupled hydraulic and mechanical system can be rigorously derived by combining the fluid mass conservation equation with the solid mass conservation equation, considering the relative motion of the fluid to the moving solid according to Rutqvist et al. (2001 [DIRS 154587]). In such a case, the volumetric strain in the mass-balance equation is coupled to the force-balance equation through Biot's storage and effective stress parameters (Biot 1941 [DIRS 121082]), and the final equations are solved simultaneously in a fully coupled model. In general, a reservoir engineering approach can be used by accounting for rock deformation changing the porosity. However, in the current application, an alternative approach of estimating change in porosity, and hence permeability, from a change in stress is used by adopting an empirical nonlinear relationship. For a fractured rock, the second approach is more direct because a relationship between fracture normal stress and fracture permeability can be used directly. Such normal stress versus fracture permeability relationships is frequently determined from laboratory tests, or can preferably be back-calculated from field tests at a relevant scale. By using this approach, the TOUGH2 V1.5 and FLAC3D V2.0 codes can be used in their standard versions, but linked together through numerically calculated porosity, permeability, and effective stress changes. The codes are executed iteratively with transfer of data through external linking modules. Through various iterative schemes, either explicit or implicit sequentially coupled solutions can be achieved.

Figure 4.3.7-5 presents the principal linkage of TOUGH2 V1.5 and FLAC3D V2.0. The two codes should be run with a mutually compatible mesh, according to Figure 4.3.7-5b. A TOUGH2 V1.5 mesh has one grid point within each grid element where temperature, fluid pressures, and saturation is defined, whereas FLAC3D V2.0 nodes are located in element corners. Thus, when transferring temperature and pressure from TOUGH2 V1.5 to FLAC3D V2.0, the data have to be interpolated from mid-element to corner nodes. No interpolation is required for the reverse data transfer from FLAC3D V2.0 to TOUGH2 V1.5 because stress and strain are defined in FLAC3D V2.0 elements, which are identical to TOUGH2 V1.5 elements.

The two codes are linked through material-specific functions (or modules) that are consistent with the continuum concepts used in both codes. In TOUGH2 V1.5, the fracture and matrix flow and interaction are modeled using a dual-permeability (overlapping continuum) concept or, alternatively, an equivalent continuum concept. In FLAC3D V2.0, an orthotropic elastic or isotropic elasto-plastic equivalent continuum model is used.

4.3.7.4.2 Application of Coupled Thermal-Hydrologic-Mechanical Continua Model to the Current Study

In this study, the joined "TOUGH-FLAC" code was applied to study the effects of the THM coupling on the flow and temperature evolution in the vicinity of a potential repository drift. The effect of the THM coupling on the fluid flow and temperature field around a drift was investigated by comparing the THM results to a pure TH simulation (i.e., using the TOUGH2 V1.5 code only). A continuum approach was used for both the TOUGH2 V1.5 part and the FLAC3D V2.0 part of the coupled code in a consistent way.

Figure 4.3.7-6a presents a schematic picture of the fractured rock system with one emplacement drift being modeled. At Yucca Mountain, the two stratigraphic units in which the emplacement drifts may be located (Tptpmn and Tptpll) are highly fractured, and the fractures are well-connected (CRWMS M&O 2000 [DIRS 153314], Section 6.7 and Figure 8). There are three dominant sets of fractures that are oriented almost orthogonal to each other, two subvertical and one subhorizontal (CRWMS M&O 2000 [DIRS 151635], Figure 5). From a TM point of view, the extensive fracturing implies that the rock is considerably softer and has a lower thermal expansion coefficient than the corresponding intact rock. However, previous simulations of TM induced displacements at the Single Heater Test and the Drift Scale Test indicate that the mechanical deformations in the rock mass can be reasonably well captured with a linear elastic or nonlinear elastic mechanical model (CRWMS M&O 1999 [DIRS 154585], Section 4.2). This is true provided that the rock mass deformation modulus and thermal expansion coefficient are reduced by about 50 percent of the value for intact rock. This implies that the bulk rock mass behavior should be essentially elastic, although locally a small slip may occur on fracture planes. Near the drift wall, on the other hand, inelastic shear slip or tensile fracturing may occur because of the strong stress redistribution and a lack of confinement in that region. The extent of this particular zone is difficult to predict because it depends on the strength parameters of the rock mass, which can only be roughly estimated.

As discussed above, because of the high density and connectivity of the fracture network, the conceptual model used is the dual-permeability model. This model is also used for the TOUGH2 V1.5 part of the coupled THM simulations described below. For the hydromechanical changes, the dominant part is the fracture continuum, where changes in the stress field will cause significant changes in fracture apertures and, hence, fracture permeability. To couple the changes in the three-dimensional stress field to the rock mass permeability, a simplified cubic block conceptual model is utilized (Figure 4.3.7-6b). In this model, the current hydraulic fracture aperture b depends on the current fracture normal stress σ_n according to the following exponential function (Bodvarsson 2001 [DIRS 154669], Attachment 9, pp. 9 and 21 to 25):

$$b = b_i + \Delta b = b_i + b_{\max}\left[\exp(\alpha\sigma_n) - \exp(\alpha\sigma_{ni})\right] \qquad \text{(Eq. 4.3.7-1)}$$

where

b_i = the initial aperture

b_{max} = the maximum aperture (at zero normal stress)

α = a parameter to be calibrated

σ_{ni} = the initial stress normal to the fractures.

Equation 4.3.7-1 and the conceptual cubic block model give the following relations for stress versus fracture permeability in three orthogonal (2 horizontal and 1 vertical) directions. In these equations, the initial fracture permeability is isotropic:

$$\frac{k_x^f}{k_i^f} = \frac{1}{2}\left[1 + \frac{b_{max}}{b_i}\left(\exp(\alpha\sigma_y) - \exp(\alpha\sigma_{yi})\right)\right]^3 + \frac{1}{2}\left[1 + \frac{b_{max}}{b_i}\left(\exp(\alpha\sigma_z) - \exp(\alpha\sigma_{zi})\right)\right]^3 \qquad \text{(Eq. 4.3.7-2a)}$$

$$\frac{k_y^f}{k_i^f} = \frac{1}{2}\left[1 + \frac{b_{max}}{b_i}\left(\exp(\alpha\sigma_x) - \exp(\alpha\sigma_{xi})\right)\right]^3 + \frac{1}{2}\left[1 + \frac{b_{max}}{b_i}\left(\exp(\alpha\sigma_z) - \exp(\alpha\sigma_{zi})\right)\right]^3 \qquad \text{(Eq. 4.3.7-2b)}$$

$$\frac{k_z^f}{k_i^f} = \frac{1}{2}\left[1 + \frac{b_{max}}{b_i}\left(\exp(\alpha\sigma_x) - \exp(\alpha\sigma_{xi})\right)\right]^3 + \frac{1}{2}\left[1 + \frac{b_{max}}{b_i}\left(\exp(\alpha\sigma_y) - \exp(\alpha\sigma_{yi})\right)\right]^3 \qquad \text{(Eq. 4.3.7-2c)}$$

The parameters in Equation 4.3.7-2 are determined as described in the next section by model calibration against a number of Yucca Mountain ESF field experiments at the scale of a drift. In addition to changes in fracture permeability, the fracture porosity is corrected for the aperture changes in Equation 4.3.7-1, and the capillary pressure varies as permeability changes according to the Leverett (1941 [DIRS 100588]) function.

For the linkage function from TOUGH2 V1.5 to FLAC3D V2.0, only the effect of thermally induced strain and stresses are considered. The changes in effective stress and bulk density caused by the multiphase fluid pressure and saturation changes are neglected. This is defensible considering that the fracture system is unsaturated, with a capillary pressure of less than 0.01 MPa. This is a very small pressure for a system that has in situ stresses and thermal stresses with magnitudes on the order of several to tens of MPa.

4.3.7.4.3 Calibration against Niche and Drift Scale Heater Tests

The parameters in the stress-permeability function (Equation 4.3.7-2) are estimated through model calibration against air-permeability measurements conducted at three excavated niches located in the Tptmn unit and one excavated niche in the Tptpll unit. The air-permeability tests measure the permeability of the fracture continuum, which is the main component controlling flux and seepage. In the Tptpmn unit, the air-permeability was measured before and after excavation in three boreholes located about 0.65 meters above the niches (DTN: LB0011AIRKTEST.001 [DIRS 153155]). The permeability was measured along each borehole in sections about 0.3 meters long, and in almost every section the permeability changed during the excavation of the niche. The ratio of post-excavation to pre-excavation permeability varies between 1.0 (no change) and approximately 1,000 (three orders of magnitude increase); on average, the permeability increased by more than one order of magnitude. Figure 4.3.7-7 presents the pre-excavation to post-excavation permeability as a function of the initial permeability in each measurement point along borehole UM, located above Niche 2 (Station 36+50) in the Tptpmn. The results indicate a general trend that permeability changes are larger in initially lower-permeability sections than in the higher-permeability sections.

Preliminary results are also available from a similar test conducted at a niche in the Tptpll unit (DTN: LB002181233124.001 [DIRS 146878]; DTN: LB0012AIRKTEST.001 [DIRS 154586]). At this niche, the air permeability was measured in boreholes above the niche and in a borehole on the side of the niche. In general, the results show that the average permeability in each borehole changed by a factor of approximately 2 to 9 above the crown of the drift (2 m from the crown) and by a factor of less than 2 on the side of the drift (1.5 to 2 m from the edge of the drift).

The stress permeability changes induced by the excavation of a niche are simulated using the FLAC3D V2.0 part of the coupled code and the stress permeability relationship in Equation 4.3.7-2. There are two parameters to be fitted in the equation, α and b_{max}. For the increase of permeability as evidenced in the niche tests, the key parameter is α. In Figure 4.3.7-7, a point noted by **x** is used as the fitting point, relating the post- and pre-excavation ion ratio (-) (i.e., k_f^j / k_i^j) with the pre-excavation permeability (m^2) (i.e., k_i^j), where k_f^j is the geometric mean of the three permeability values in the x, y, and z directions computed from Equation 4.3.7-2.

Next, a calibration of the fracture residual aperture residual aperture (i.e., the limiting aperture remaining after compressive stresses induced by excavation and heating have closed the fracture as far as possible), which is related to b_{max} in Equation 4.3.7-2, was conducted against air-permeability measurements in the Drift Scale Test. Those measurements (CRWMS M&O 2000 [DIRS 151964]) showed that the air permeability near the drift decreased at most by a factor of 0.1 during heating. This permeability decrease may be caused partly by an increase in liquid fracture saturation and partly by mechanical fracture closure from TM effects. A conservative approach for the THM calculation is to take the measured reduction in permeability as caused entirely by TM effects, probably overestimating the TM effects. Therefore, the residual aperture was calibrated to limit the permeability changes during closure to 0.1. This is an important parameter in the simulations.

For confirmation, Figure 4.3.7-8 (left) presents the distribution of permeability changes calculated from a calibrated model in the Tptpmn unit. In this figure, the permeability before and after excavation has been calculated from the geometric mean of the anisotropic permeability values in three directions. The calculated permeability values at borehole UM are calibrated to a permeability change of 20, which is in the middle range for pre-excavation to post-excavation changes for the corresponding initial permeability (3.7×10^{-13} m^2) in Figure 4.3.7-7. Figure 4.3.7-8 (right) shows the simulated excavation induced permeability changes in the Tptpll unit. In this case, the same parameters for the hydromechanical function are used, with the exception of the initial permeability. Because the initial permeability is higher in the Tptpll rock unit (2.4×10^{-12} m^2), the change in permeability is smaller than the changes in the Tptpmn unit. The simulation results in these figures are consistent with the observed data in both the Tptpmn and Tptpll units.

4.3.7.4.4 Application and Results of the Coupled Thermal-Hydrologic-Mechanical Model

A fully coupled THM simulation using the explicit solution scheme was conducted on a one-half symmetric drift located at Yucca Mountain (Figure 4.3.7-9). The model domain is a multiple-layered column extending vertically from the ground surface down to the water table. The vertical layering for the model was chosen to correspond to the vertical contacts at Nevada State Plane Coordinates 170572.39 m (Easting) and 233194.536 m (Northing), with corresponding geologic contacts for the three-dimensional UZ site-scale model 1999 TSPA grid (DTN: LB990701233129.001 [DIRS 106785]; CRWMS M&O 2000 [DIRS 114277], Attachment VI). The hydrologic and thermal properties of the layers are taken from the drift scale calibrated property sets (DTN: LB0011DSTFRAC1.001 [DIRS 153470]; DTN: LB990861233129.001 [DIRS 110226]). The ground surface boundary was set at constant temperature and mechanically free, and the water table boundary at constant temperature and mechanically fixed. By symmetry, only half of the distance between two drifts (40.5 m) was modeled because the drift spacing is 81 m. A drift of 5.5-m diameter was simulated as being excavated in the Tptpll unit. The drift was treated as a single element with a porosity near one and a mechanically free boundary. The waste emplacement was designed such that two thermal operating modes were simulated. The first is referred to as the higher-temperature or above-boiling case, in which a heat input of 1.45 kW/m of drift is applied with a forced ventilation period of 50 yrs, during which 70 percent of the decay heat is removed. The second is referred to as the lower-temperature or below-boiling case, in which a heat input of 1.35 kW/m of drift is applied with a forced ventilation period of 300 yrs, during which 80 percent of the decay heat is removed. Details of these input scenarios and updated thermal parameters are discussed in Section 4.3.5. The THM parameters are shown in Table 4.3.7-4, including the calibrated parameters α and b_{max}.

Results of the fully coupled THM continua model analysis are shown in the next series of figures (Bodvarsson 2001 [DIRS 154669], Attachment 9, pp. 32 to 76).

Figure 4.3.7-10 shows the changes in vertical and horizontal permeability around the drift because of excavation. There is a significant increase by a factor up to 10 in rock permeability above the crown of the drift. Near the springline of the drift, vertical permeability is increased but horizontal permeability is decreased, resulting in much smaller changes in mean permeability. Note that the complex pattern of changes is obtained by calculating permeability in a given direction by combining two permeability values in the two fracture directions parallel to it (see Equation 4.3.7-2).

Figure 4.3.7-11 shows the temperature distribution at 10 yrs for the HTOM and LTOM. As expected, the temperature increase centers around the drift, and the disturbance is more pronounced in the higher-temperature case. Figures 4.3.7-12 and 4.3.7-13 present changes in the horizontal and vertical permeabilities (respectively) after 10 yrs. On the whole, there is a decrease in permeability around the drift caused by thermal stress induced by the decay heat.

This decrease is able to overcome the initial excavation-induced permeability increases, except possibly in areas very close to the crown of the drift. Changes in both cases are similar.

Figure 4.3.7-14 shows the temperature distributions at 1,000 yrs for the higher-temperature and lower-temperature cases. The differences are apparent. In the former, temperatures near the drift are still above boiling, and temperatures at about 80 m above the drift are over 80°C. In the latter, temperatures are 20° to 40C° lower, and at 80 m above the drift the temperature is about 60°C. Figures 4.3.7-15 and 4.3.7-16 show the changes in horizontal and vertical permeabilities at 1,000 yrs. There is a trend of little or no change in permeability in the lower lithophysal layer near the drift, to a larger change 10 to 60 m above the drift, to the largest change (k_h/ki is about 0.5 and k_v/h_i is about 0.1) in the layer about 65 to 85 m above the drift (1,145 to 1,165 m section in the figure), to less change in the layer above.

The largest change, at the 1,145- to 1,165-m level, is due first to the initially lower permeability of the Tptpmn, which will experience a larger change factor due to stress changes. This is consistent with the niche calibration data discussed in Section 4.3.7.4.3. In that case, the stress change results from excavation, while in this case the stress change results from temperature rise. Secondly, the shallower layers above the drift, which have less overburden, will respond to stress changes more readily (i.e., the effective rock stiffness is relatively less).

An interesting observation is that these changes are almost the same regardless of the operating mode. The change of k_v/ki = 0.1 indicates that the thermal stress has caused a reduction of fracture permeability to the residual value. This is true even in the LTOM, so a higher-temperature cannot induce additional changes. The residual permeability was estimated by calibration against the Drift Scale Test (see Section 4.3.7.4.3), where a reduction of air-permeability values to 0.1 of their initial values was observed. As discussed in Section 4.3.7.4.3, this reduction could be due to a combination of TM effects and relative permeability change with saturation. Attributing it all to the TM effect is a conservative limit for THM evaluation. If the TM part of the change had been chosen not at this full value, the results in these figures would show less permeability reduction. Thus, the residual permeability value of the formation and the stiffness of the formation at Yucca Mountain are important parameters for the evaluation of THM processes. A reevaluation of field observations at Yucca Mountain and, in particular, the on-going Drift Scale Test will be of paramount importance.

The saturation and percolation flux distributions at 1,000 yrs with and without THM coupling are shown in Figures 4.3.7-17 and 4.3.7-18 for the higher- and lower-temperature cases, respectively. The main difference in saturation profiles between TH and THM results is the higher saturation in the Tptpmn unit at the 1,145- to 1,165-m level. This corresponds to the THM induced reduction in permeability, with a corresponding increase of capillarity in this layer. The liquid flow patterns, on the other hand, are quite similar between the TH and THM cases. The reduced permeability in the 1,145- to 1,165-m zone is accompanied by a higher relative permeability from the increased liquid saturation, which may have compensated for part of its impact. Another reason for similarity in liquid flux patterns may be that permeability reduction is constant horizontally across the flow domain; the vertical downward flux cannot flow around regions of reduced permeability, and is thus forced to take the same flow pattern. Therefore, the percolation fluxes immediately above the drift appear to be very similar for both the TH and THM results.

The following conclusions may be drawn from the coupled THM continua analysis:

- The fully coupled THM model has been calibrated against ESF niche and Drift Scale Test data. During drift excavation, permeability above and below the drift is expected to increase by one order of magnitude or more, while permeability to the side of the drift is expected to have much smaller changes.

- With waste emplacement and thermal input, thermal stress will reduce permeability all around the drift. Although this reduction is relative to the initial excavation-induced permeability increase, there is a net permeability decrease after about one year of heating.

- In the longer term, after around 1,000 yrs, thermal effects will cause permeability changes far from the drift (up to 100 m). Except in the region very close to the drift walls, there is permeability reduction caused by thermal stress, with most changes in the vertical permeability. The reduction is a function of initial local permeability values, being larger for initially low values. The reduction is large enough so that the permeability at 1,000 yrs in the Tptpmn unit about 60 m above the drift will reduce to its residual value (i.e., permeability at residual aperture).

- Rock stiffness parameters and residual permeabilities are important parameters for the THM analysis, which suggests additional testing and further analysis of Drift Scale Test data may be needed.

4.3.7.4.5 A Discussion of Permanent Permeability Changes Due to Thermal-Hydrologic-Mechanical Processes

Part of the permeability changes induced by the excavation and heating of the rock could remain after the repository has cooled to the ambient temperature. Such permanent changes are important for a performance assessment of a repository. In the simulations presented in this section, permanent changes are induced as results of drift excavation. These changes are as much as an order of magnitude in a zone near the drift that extends from the drift wall into the rock for about one drift radius. The subsequent heating and cooling of the rock mass did not induce any significant permanent changes in the permeability field in these simulations. The permeability change during the heating of the rock was induced by a predominant elastic closure of rock fracture, but after cooling these changes would be diminished by an elastic, fully reversible recovery of fracture apertures. Thus, a permanent permeability change would not result unless the rock mass behaved inelastically. The most significant inelastic behavior is likely to occur in the form of shear slip and tensile failure along preexisting fracture planes and in the inelastic zone near the drift. Such inelastic behavior would tend to increase the permeability in this zone; at the same time, a general non-recoverable redistribution of the stress field around the drift would cause small changes in the permeability field outside the inelastic region. Furthermore, even if the rock mass behavior away from the drift wall is essentially elastic as a whole, local inelastic behavior may occur, for example, in the form of fracture slip and crushing of asperities during fracture compression. Such small-scale inelastic behavior may not be significant for the general deformation of the rock mass as measured by extensometers, but may still be significant for the local fracture aperture and thus the local fracture permeability.

In the Single Heater Test, a small stick-slip displacement behavior was observed by extensometers during the cooling phase, which could be interpreted as fracture slip phenomenon. Permanent displacements of up to 1 mm occurred in the rock near the heat source and at the drift walls. Furthermore, a permanent general increase in the permeability field by a factor of up to 3.5 was observed in the Single Heater Test area. These permanent permeability changes occurred during the heating and cooling of the rock mass and may be caused by permanent mechanical opening of fractures. Further information on permanent changes will be available after the completion of the Drift Scale Test. A careful analysis of test data will be very important to shed light on this issue.

4.3.7.5 Abstraction for Total System Performance Assessment

The work reported in this section is devoted to evaluating process model sensitivities and uncertainties. Simulation results from this study are not yet used to support any abstraction model that directly supports a TSPA. The results found so far indicate that percolation flux values and distribution immediately above the drift are not significantly affected by the THM processes. Further, permeability changes caused by THM effects, apart from the immediate neighborhood of the drift that is part of the drift degradation analysis (see Section 4.3.4), are about one order of magnitude, which is within the range of the ambient seepage model (see Section 4.3.4). Thus, results to date do not indicate a significant THM induced impact on the performance as represented in the total system performance baseline.

4.3.7.6 Multiple Lines of Evidence

The impact of THM processes (such as excavation and heating) on the performance of the potential repository at Yucca Mountain have been assessed through field studies at a variety of underground sites. These studies indicate that the effects of excavation on rock stability tend to be highly site-specific, depending on rock physical properties, the presence and orientation of faults and fractures, and the local stress regime. Excavation often leads to localized increases in permeability. Heating generally results in an increase in stress and a reduction in permeability due to thermal expansion. The results of THM experiments conducted at the Nevada Test Site and the Stripa underground laboratory in Sweden are summarized below.

4.3.7.6.1 Nevada Test Site Thermal-Hydrologic-Mechanical Experiments

Four TM/THM experiments relating to high-level nuclear waste research were conducted at the G-tunnel in Rainier Mesa. These tests included a single borehole heater test, a small-diameter heater test, a heated block test, and a prototype engineered barrier system field test. One objective of the heated block test was to measure rock mass mechanical and TM properties of ash-flow tuff under controlled thermal and stress loading conditions. The block was subjected to maximum temperatures ranging from 76° to 130°C and equal biaxial stresses with magnitudes up to 10.6 MPa (Zimmerman et al. 1986 [DIRS 145625]). The effective modulus of deformation ranged from 0.4 to 0.83 times the intact rock measurements, depending on the number of joints included and their apertures. A slight dependence of modulus on stress was indicated, but no significant temperature effects on modulus were identified.

A second objective of the heated block test was to determine the effects of excavation, stress, and temperature changes on the permeability of a single joint. The permeability of a single near-vertical fracture was measured using three vertical boreholes in a linear array. The largest changes in permeability were associated with excavation of the block, when the apparent permeability increased from 76×10^{-12} m^2 to 758×10^{-12}m^2. Subsequent compressive loading decreased the permeability but did not completely reverse the unloading conditions, and the apparent permeability ranged from 252×10^{-12} m^2 to 332×10^{-12} m^2 microdarcies over a stress range of 3.1 to 10.6 MPa (Zimmerman et al. 1986 [DIRS 138273], p. ix and Section 11). Increased temperature under biaxial confinement decreased the fracture aperture, lowering the apparent permeability from 234 to 89 microdarcies during heating caused by thermal expansion of the rock. These observations are consistent (of the same order of magnitude) with the Yucca Mountain THM modeling and field studies described earlier.

4.3.7.6.2 Underground Testing at Stripa

A time-scaled heater test was performed at Stripa to investigate the long-term TM response to thermal loading (Chen et al. 1980 [DIRS 154672]). Analysis showed that, in the full-scale and time-scale heater tests, heat flow conformed to linear conduction theory and was not affected by fractures or other discontinuities. Thermoelastic deformation of the rock mass was nonlinear and less than expected. Early in the tests, measured displacements were much less than predicted by linear thermoelasticity. Later, the displacements increased uniformly, but in fixed proportions to predicted levels. This was likely a result of the closing of fractures in response to thermal expansion. Fracture closure was confirmed by observation of diminished water inflow to the heater and instrument boreholes (Nelson et al. 1981 [DIRS 150092]) and by increased compressional wave velocity during heating (Paulsson et al. 1980 [DIRS 154570]). The closing of fractures (and resulting changes in fracture permeability due to thermal input) is consistent with the results of the Yucca Mountain studies described in this section.

4.3.7.6.3 Geothermal Reservoir Temperature-Permeability Correlation

In addition to field studies of coupled THM processes that provide direct evidence of how a potential repository at Yucca Mountain would perform, corroborative results on coupled THM effects may be found in the geothermal literature. A survey of geothermal reservoir properties worldwide (Björnsson and Bodvarsson 1990 [DIRS 154606]) showed a correlation between permeability and temperature for various geothermal systems (Figure 4.3.7-19). The values are scattered, but they indicate a trend toward decreasing permeability with increasing temperatures. The low permeability at temperatures around 300°C and above is more likely caused by geochemical effects. The THM effects may be present at lower temperatures. The straight-line fit through the points has a regression coefficient of 0.5 and shows a half-order decrease in permeability with a 100C° increase in temperature (Bodvarsson 2001 [DIRS 154669], Attachment 4, p. 36).

4.3.7.7 Summary of Uncertainties and Their Treatment

Table 4.3.7-5 provides a summary of the uncertainty issues related to THM effects on seepage and their treatment.

4.3.7.8 Summary and Conclusions

Two alternative conceptual and numerical models have been used to study the impact of coupled THM processes on potential seepage into drifts: the distinct-element model and the fully coupled THM continua model. Two thermal operation modes were also considered, one with above-boiling temperatures near the repository and the other with below-boiling temperatures. Detailed results on stresses, deformations, and changes in permeability at a series of times after waste emplacement have been calculated. While significant changes may be found very close to the drift walls (covered by drift degradation scenarios), permeability changes may be about one order of magnitude; a comparison of percolation fluxes and saturation about 20 m directly above a drift in the Tptpll unit do not show much difference between the fully coupled THM and purely TH cases. Thus, the results so far do not require adjustments in seepage estimates already in the TSPA baseline (CRWMS M&O 2000 [DIRS 153246]).

Two models are presented to evaluate uncertainties and the effect of different thermal operating modes. A distinct element analysis representing a two-way TM coupled analysis is presented in Section 4.3.7.3. Using temperatures imported from a multiscale thermal model at discrete time intervals, the results of the distinct element analysis concludes heating associated with waste emplacement will cause drift walls to displace inward as horizontal stress levels increases. Model results predict fracture permeability will increase substantially in the first 2 m of rock around the emplacement drift. The distinct element model also predicts fracture permeability will increase in the region above the drift, extending to one drift diameter above the drift wall (see Section 4.3.7.3.3). Increases in permeability greater than one order of magnitude are not predicted beyond 0.5 m from the drift, except in the region above the drift (see Section 4.3.7.3.3). Beyond the immediate zone of increased permeability, permeability is substantially reduced in vertical fractures, leading to an overall reduction in permeability (see Section 4.3.7.3.3, Bullet 2).

A coupled THM continua model calibrated against ESF niche data and the Drift Scale Test is consistent with available data (see Section 4.3.7.4.1). With waste emplacement and thermal input, the coupled model predicts thermal stress will reduce permeability all around the drift (see Section 4.3.7.4.4, Bullet 2). Although this reduction is relative to the initial excavation-induced permeability increase, there is a net permeability decrease after about one year of heating. In the longer term, thermal effects will cause permeability to change far from the drift (up to 100 m), with most change occurring in the vertical permeability. Permeability reduction is a function of initial local permeability values, being larger for initially low values.

While the results of these two approaches predict permeability reductions in the elastic regions away from the drift wall, there are apparent contradictory results at the drift wall: there is an increase in permeability in the distinct element analysis, but there is a decrease in permeability in the continuum analysis. These contradictions are caused by different model conceptualizations and are affected by local fracture and rock mass strength parameters. Because this region is near a free surface, a distinct element model provides more freedom of block movements along fracture planes, while such movements are prevented in the continuum model. This difference in simulation results may have an effect on the immediate neighborhood of the drift that is part of the drift degradation analysis (see Section 4.3.4).

Permanent changes in permeability are the results of inelastic rock behavior (see Section 4.3.7.4.5). The only inelastic strain to be expected is from shear displacement along preexisting fractures. This transitional behavior between elastic and inelastic behavior may occur during heating and cooling. The continuum THM model predicts no significant inelastic behavior, while the distinct element model predicts significant inelastic behavior and permanent changes near the drift wall. Outside the potentially inelastic region near the drift wall (which is part of the drift degradation analysis; see Section 4.3.4), the nonlinear inelastic behavior of the rock may be insignificant, as results from the Single Heater Test and Drift Scale Test indicate (see Section 4.3.7.4.2). However, the distinct element modeling (see Section 4.3.7.3.3) indicates a permanent permeability increased in regions away from the drift wall in the case of a high heat load. Further information on potential permanent changes in permeability will be available after the completion of the Drift Scale Test.

The permeability decreases caused by THM effects, apart from the immediate neighborhood of the drift that is part of the drift degradation analysis, are about one order of magnitude, which is within the range of the ambient seepage model (see Sections 4.3.4 and Section 4.3.7.5). Permeability increases predicted by the distinct element model are also within the range of the ambient seepage model. Consequently, the results so far indicate that percolation flux values and distribution above the drift are not significantly affected by THM processes not already captured by drift-scale degradation. The results do not indicate a significant TM or THM induced impact on repository performance that would change the results of the uncoupled TH analysis supporting the TSPA-SR (CRWMS M&O 2000 [DIRS 153246]; see also Section 4.3.7.5). In terms of performance, the evaluation of thermal operating modes suggests they have little effect on the THM responses on the rock beyond what has been captured in the TSPA-SR.

A number of uncertainties have been addressed in this section; however, many still remain, some of which are indicated in Table 4.3.7-5. A comprehensive comparison between the distinct-element model results and results from the fully coupled THM continua model has not yet been done. Though the coupled THM continua model has been calibrated against available data from the niche excavation tests and the Drift Scale Test, more comprehensive calibration studies are still needed. In particular, rock stiffness with respect to thermal stresses and the residual permeability values of the geological layers above the drift are important parameters for modeling THM impact. Finally, how heterogeneity in the initial permeability field around a drift interfaces with coupled THM processes in affecting the potential for drift seepage also needs to be addressed.

Table 4.3.1-1. Triangular Distributions of Seepage Fraction, Seep Flow Rate, and Standard Deviation of Seep Flow Rate as a Function of Percolation Flux

q (mm/yr)	Minimum of Triangle (Low-Seepage Case)			Peak of Triangle (Base Case)			Maximum of Triangle (High-Seepage Case)		
	f_s	Mean Q_s (m^3/yr)	Std. Dev. Q_s (m^3/yr)	f_s	Mean Q_s (m^3/yr)	Std. Dev. Q_s (m^3/yr)	f_s	Mean Q_s (m^3/yr)	Std. Dev. Q_s (m^3/yr)
2.4	0	0	0	0	0	0	0	0	0
5	0	0	0	0	0	0	8.31×10^{-2}	8.57×10^{-2}	3.95×10^{-2}
14.6	0	0	0	0	0	0	8.31×10^{-2}	0.401	9.55×10^{-2}
60.0	0	0	0	0	0	0	0.310	0.701	0.815
73.2	6.60×10^{-3}	0.365	7.99×10^{-2}	5.41×10^{-2}	0.365	7.99×10^{-2}	0.376	0.788	1.02
213	6.60×10^{-3}	3.99	0.210	5.41×10^{-2}	4.24	0.210	0.452	4.24	2.34
500	7.65×10^{-2}	1.56	3.94	0.129	6.20	5.39	0.512	12.1	6.89
1000	0.261	27.1	16.1	0.303	30.9	17.3	0.609	35.6	18.5
3000	1	129	64.7	1	129	64.7	1	129	64.7

Source: Based on CRWMS M&O 2001 [DIRS 154291], Table 16.

Table 4.3.1-2. Summary of Uncertainty Issues Related to the Determination of Seepage-Relevant Parameters

Category	Uncertainty Issue	Treatment of Uncertainty Issue	Affected Goals
Conceptual uncertainties	Drift acting as capillary barrier	Based on unsaturated flow theory (Philip et al. 1989 [DIRS 105743]) Implemented through choice of unsaturated flow process model (Section 4.2.2; CRWMS M&O 2001 [DIRS 153045], Section 5) Confirmed through reproducibility (calibration) and prediction (validation) of seepage test data (CRWMS M&O 2001 [DIRS 153045], Sections 6.3.4 and 6.4.4) Corroborated by direct observations and natural analog studies (Section 4.3.1.7) Alternative conceptual models examined (CRWMS M&O 2001 [DIRS 153045], Section 6.5)	Development of general understanding of seepage process and basis for seepage prediction models
	Ability of model to predict seepage under natural percolation conditions (validity of extrapolation assumption)	Demonstrated ability to predict seepage tests in validation exercise (CRWMS M&O 2001 [DIRS 153045], Sections 6.3.4 and 6.4.4) Examined extrapolation to natural conditions in theoretical study (Finsterle 2000 [DIRS 151875])	Seepage predictions for waste emplacement drifts using calibrated model
	Significance of microfractures, film flow, small-scale surface roughness	Accounted for through estimation of effective parameters in seepage experiment (Section 4.3.1.3; CRWMS M&O 2001 [DIRS 153045], Section 6.1.6)	Determination of seepage-relevant parameters

Table 4.3.1-2. Summary of Uncertainty Issues Related to the Determination of Seepage-Relevant Parameters (Continued)

Category	Uncertainty Issue	Treatment of Uncertainty Issue	Affected Goals
Conceptual uncertainties (Continued)	Role of excavation-disturbed zone (EDZ)	Seepage test conducted within EDZ to directly obtain EDZ-related parameters relevant for seepage (Section 4.2.3)	Determination of seepage-relevant parameters
Data uncertainties	Evaporation losses prior to and during liquid-release tests	Assumed to be insignificant (CRWMS M&O 2001 [DIRS 153045], Sections 5.6 and 7.4) Partly accounted for in calibration of Tptpll data (CRWMS M&O 2001 [DIRS 153045], Section 6.3.3.2) Addressed in future seepage tests through humidity control and monitoring	Determination of unbiased parameters
	Storage and memory effect	Accounted for through simulation of actual test sequence during inversion (CRWMS M&O 2000 [DIRS 119412], Section 6.4) Mitigated by conducting long-term seepage experiments (CRWMS M&O 2001 [DIRS 153045], Section 6.1.6)	Determination of unbiased parameters
	Random measurement errors	Accounted for in error analysis (CRWMS M&O 2001 [DIRS 153045], Table 11)	Determination of parameter uncertainty
Parameter uncertainties	Formation-specific parameters	Seepage tests performed in Tptpmn and Tptpll to obtain unit-specific, seepage-relevant parameters (CRWMS M&O 2001 [DIRS 153045], Sections 6.3 and 6.4) Determined average properties and measure of variability (CRWMS M&O 2001 [DIRS 153045], Table 11)	Determination of seepage-relevant parameters
	Heterogeneity	Use of heterogeneous seepage models (CRWMS M&O 2001 [DIRS 153045], Sections 6.3.2 and 6.4.2; CRWMS M&O 2000 [DIRS 153314], Section 6.3) Calibration and prediction partly based on multiple realizations of permeability field (CRWMS M&O 2001 [DIRS 153045], Sections 6.3.3.3; CRWMS M&O 2000 [DIRS 153314], Section 6.3) Standard deviation increased in seepage abstraction (CRWMS M&O 2001 [DIRS 154291], Section 6.2)	Distribution of seepage-relevant parameters
	Uncertainty propagation	Stochastic data uncertainty reflected in estimation uncertainty (CRWMS M&O 2001 [DIRS 153045], Table 11) Deterministic seepage predictions over entire range of potential parameter values as basis for probabilistic sampling (CRWMS M&O 2000 [DIRS 153314], Section 6.6) Parameter distributions developed based on estimation uncertainties and variability measures (CRWMS M&O 2001 [DIRS 154291], Section 6.2) Distribution of other input parameters (e.g., percolation flux) developed based on deterministic runs and sensitivity analyses (CRWMS M&O 2001 [DIRS 154291], Sections 6.2 and 6.3) Linear uncertainty propagation analyses and Monte Carlo simulations performed as part of model validation (CRWMS M&O 2001 [DIRS 153045], Sections 6.3.4 and 6.4.4)	Distribution of parameters in TSPA calculation

Table 4.3.2-1. Cases Considered in Flow Focusing Sensitivity Studies

Realization	Infiltration (mm/yr)	Infiltration Pattern	Correlation Length for Fracture Permeability (m)
Realization #1	1 to 500	Uniform	1
Realization #2	1 to 500	Uniform	1
Realization #3	1 to 500	Uniform	3
Realization #4	5	Spatial Pulse/5 m	1

Table 4.3.2-2. Summary of Uncertainty Issues Related to Flow Focusing and Discrete Flow Paths in the TSw Hydrogeologic Unit

Category	Uncertainty Issue	Treatment of Uncertainty Issue	Affected Goals
Conceptual uncertainties	Representation of multiscale flow focusing	Large-scale flow redistribution captured in mountain-scale model Intermediate-scale flow focusing addressed through flow focusing factors in abstraction Small-scale flow focusing explicitly accounted for in heterogeneous drift-scale model	Percolation distribution for seepage models
	Development of flow channels	Mountain-scale model assumes homogeneous hydrostratigraphic units Percolation calculation in high-resolution, stochastic permeability field	Simulating intermediate-scale channel development
	Validity of weeps model, active fracture model, and stochastic fracture continuum model	Weeps model used to obtain upper limit of weep spacing in seepage abstraction Active fracture model used to obtain lower limit of weep spacing in seepage abstraction Sensitivity analyses of effect of fracture/matrix interaction on flow focusing	Determination of flow focusing factors for seepage abstraction
	Role of lithophysal cavities	Lithophysal cavities included in seepage model Accounted for through estimation of effective parameters	Small-scale flow focusing
	Role of PTn	PTn assumed to dampen spatial and temporal flow focusing Transient simulations performed for locations without PTn	Assessment of steady-state assumption
Data uncertainties	Observing or testing preferential flow	Continue weep observations in Niche 5 and others Chlorine-36 observations and analyses in ESF Analyze observed saturation and water potential distributions to derive weep spacing Analogue studies from appropriate sites	Validating flow focusing model

Table 4.3.2-2. Summary of Uncertainty Issues Related to Flow Focusing and Discrete Flow Paths in the TSw Hydrogeologic Unit (Continued)

Category	Uncertainty Issue	Treatment of Uncertainty Issue	Affected Goals
Parameter uncertainties	Parameters for generating stochastic fracture permeabilities for the TSw hydrogeologic units above the potential repository horizon	Determined through calibration against pneumatic and air-permeability data	Determination of flow focusing and distribution of weep spacing
	Matrix effects	Must be evaluated through sensitivity studies	Fracture and matrix flow components of focused flow

Table 4.3.3-1. Summary of Uncertainty Issues Related to Rock Bolts

Category	Uncertainty Issue	Treatment of Uncertainty Issue	Affected Goals
Conceptual uncertainties	Rock bolt condition	Detailed simulations conducted for various rock bolt properties (intact, grouted, and empty hole)	Impact of rock bolts on seepage
	Flow into and out of rock bolt hole	Detailed simulations conducted Sensitivity analyses performed regarding potential of backflow from rock bolt into formation Conservative simulation performed with maximum inflow into and no outflow from rock bolt	Impact of rock bolts on seepage
Data uncertainties	Observation of dripping from rock bolts	Discussed alternative conceptual models explaining observed dripping from rock bolts	Validating rock bolt model
Parameter uncertainties	Parameters of rock bolts	Performed sensitivity analysis for large range of rock bolt properties	Determination of seepage increase due to rock bolts

Table 4.3.4-1. Seepage Percentage for Alternative Drift-Degradation Scenarios for Qp = 500 mm/yr and Set A

Condition	Seepage Percentage		
	R1	R2	R3
No-degradation case	7.1	7.1	13
1 m rockfall from crown of drift	7.2	7.3	12
1m rockfall from springline of drift	7.1	7.1	13
3 m rock failure in drift roof	9.0	11	15

Source: CRWMS M&O 2000 [DIRS 153314], Table 12.

Table 4.3.4-2. Seepage Percentage for Set A Drift Degradation Scenarios

Q_p (mm/yr)		14.6	73.2	213.4	500
Base Case	R1	0.0	0.0	0.46	5.69
	R2	0.0	0.0	0.82	11.04
	R3	0.0	0.0	0.15	10.71
	Average	0.0	0.0	0.48	9.15
Worst Case	R1	0.0	0.0	0.48	8.97
	R2	0.0	0.0	0.86	13.99
	R3	0.0	0.0	0.34	12.58
	Average	0.0	0.0	0.56	11.85
75% Case	R1	0.0	0.0	2.87	10.63
	R2	0.0	0.0	3.39	17.53
	R3	0.0	0.0	2.36	16.50
	Average	0.0	0.0	2.87	14.89

Source: TerBerg 2001 [DIRS 155032].

Table 4.3.4-3. Seepage Percentage for Set B′ Drift Degradation Scenarios

Q_p (mm/yr)		500	1000	1500	2000	2500
Base Case	R1	0.0	0.0	0.33	0.55	0.83
	R2	0.0	0.0	0.50	1.05	2.09
	R3	0.0	0.0	0.0012	1.03	2.86
	Average	0.0	0.0	0.28	0.88	1.93
Worst Case	R1	0.0	0.2	0.65	1.42	2.41
	R2	0.0	0.0	1.50	3.04	4.56
	R3	0.0	0.0	0.11	1.94	4.25
	Average	0.0	0.07	0.75	2.13	3.74
75% Case	R1	0.0	0.0	0.33	0.59	1.24
	R2	0.0	0.0	0.50	1.06	2.32
	R3	0.0	0.0	0.33	1.36	3.10
	Average	0.0	0.0	0.39	1.00	2.22

Source: TerBerg 2001 [DIRS 155032].

Table 4.3.4-4. Summary of Uncertainty Issues Related to Determining Seepage-Relevant Parameters

Category	Uncertainty Issue	Treatment of Uncertainty Issue	Affected Goals
Conceptual uncertainties	Frequency and geometry of rockfalls	Used 3-D drift geometry from detailed rockfall analyses based on a rock-mechanics code and in situ fracture geometric data	Impact of rockfall on seepage
Data uncertainties	Seepage data from degraded drift	Seepage-relevant parameters obtained by calibration include effects of roughness Calibrated model used to simulate seepage into degraded drift	Validating seepage model
	Rockfall data	Observation in ESF and other tunnels and cavities	Validating rockfall model
Parameter uncertainties	Seepage-relevant parameters	Simulations performed with best-estimate parameter set of Tptpmn and Tptpll Sensitivity analyses performed for various percolation fluxes	Determining seepage increase from drift degradation

Table 4.3.5-1. Analysis Model Report Revision 00 and Post-Analysis Model Report Lithophysae Thermal Property Values

Unit	AMR Thermal Property Values			Lithophysae Thermal Property Values		
	C_R J/(kg °K)	λ_{wet} W/m °K	λ_{dry} W/m °K	C_R^* J/(kg °K)	λ wet, with lithophysae W/m °K	λ dry, with lithophysae W/m °K
Tptpul (TSw33)	882.5	1.683	0.79	657.2	1.55	0.84
Tptpmn (TSw34)	948	2.33	1.56	948	2.33	1.56
Tptpll (TSw35)	900	2.02	1.2	770.5	1.87	1.27

Source: Bodvarsson 2001 [DIRS 154669], Attachment 17, pp. 46 to 48.

Table 4.3.5-2. Statistical Parameters Used in the Three-Dimensional Heterogeneous Line-Averaged-Heat-Source, Drift-Scale Thermohydrologic Model Realizations

Stochastic Realization	Standard Deviation of *k* ($\log_{10}$)	Correlation Length (m)			van Genuchten Alpha Value Correlated to *k*
		Lateral (x)	Longitudinal (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 154985], Table 6-8.

Table 4.3.5-3. Input Parameters for Application of Asperity-Induced Episodic Infiltration at Yucca Mountain

Input Parameter	Value/Distribution	Basis/Reference
Fracture storage aperture, b_1 [m]	Assumed log-normal distribution $\mu_{ln(b1)} = -6.3$ $\sigma_{ln(b1)} = 0.48$	Mean aperture for TSw34, TSw35, and TSw36 from CRWMS M&O 2000 [DIRS 141418], Table 3. Standard deviation from CRWMS M&O 2000 [DIRS 141418], Table 4, last row, 6th column; DTN: SN0005T0581699.005 [DIRS 151514]. Values, originally in log space, were converted to natural log space for use in Mathcad 7.
Fracture pinch-point aperture, b_2 [m]	Assumed log-normal distribution $\mu_{ln(b2)} = -9.2$ $\sigma_{ln(b2)} = 0.48$	Mean log aperture calculated using Equation 27 and values in CRWMS M&O 2000 [DIRS 141418], Table 4, 6th row, 1st - 4th columns. Standard deviation from CRWMS M&O 2000 [DIRS 141418], Table 4, last row, 6th column; DTN: SN0005T0581699.005 [DIRS 151514]. Values originally in log space were converted to natural log space for use in Mathcad 7.
Width of individual weep, *w* [m]	Varied from 0.001 to 1	These limits bound values of weep widths observed by Kneafsey and Pruess 1998 [DIRS 145636] and Nicholl et al. 1994 [DIRS 141580].
Spacing between weeps, *a* [m]	Uniform distribution between log values of -0.14 and 1.78 (log-uniform distribution in real space)	The limits of the distribution are calculated by taking one standard deviation below and above the lower- and upper-bound log of the means, respectively, as given in CRWMS M&O 2001 [DIRS 154291], Section 6.4.3, Table 15; DTN: SN0012T0511599.003 [DIRS 153688], which calculated flow focusing effects using results from three-dimensional UZ flow models.
Dynamic viscosity, μ [kg/m-s]	4.89×10^{-4}	Calculated at average temperature for subboiling conditions at (20+96)/2=58°C (Incropera and DeWitt 1985 [DIRS 100623], Table A.6).
Surface tension, σ [N/m]	0.067	Calculated at average temperature for subboiling conditions at (20+96)/2=58°C (Incropera and DeWitt 1985 [DIRS 100623], Table A.6).
Liquid density, ρ [kg/m^3]	984 (used for sub-boiling conditions) 961 (used for boiling conditions)	Subboiling value calculated at average temperature of (20+96)/2=58°C. Boiling value calculated at 96°C (Incropera and DeWitt 1985 [DIRS 100623], Table A.6).
Heat of vaporization, h_{fg} [J/kg]	2.27×10^6	Calculated at 96°C (Incropera and DeWitt 1985 [DIRS 100623], Table A.6).
Extent of boiling front from drift center [m]	Assumed uniform distribution from 2.75 to 7.95	The lower value of the distribution is based on the drift radius; the upper value is the average maximum boiling extent calculated from 610 locations (DTN: LL000509112312.003 [DIRS 150798]). The superheated distance to the drift wall, *d*, is calculated by subtracting 2.75 m from the resulting distribution.
Thermal diffusivity, α [m/s^2]	5.25×10^{-7}	Value calculated by dividing thermal conductivity of dry rock (1.2 W/m-K) by rock-grain density (2540 kg/m^3) and rock-specific heat (900 J/kg-K) (DTN: SNT05071897001.012 [DIRS 106089]).
Heat load, *Q* [W/m]	148	The source data are from DTN: SN9907T0872799.001 [DIRS 111485] (see "DRFT-Scale 2-D models" worksheet in Excel file "heat TSPA-SR--9918.4-Ta.xls"). These data are multiplied by 0.94131 per CRWMS M&O 2000 [DIRS 149862], p. 83, and then an average heat generation [W/m] is calculated for 1000 years with 70% energy removal for 50 years. This is calculated by integrating the resulting heat generation curve for 1,000 years (Kaleidagraph v. 3.5.1) and then dividing the area by 1,000 years.

Table 4.3.5-3. Input Parameters for Application of Asperity-Induced Episodic Infiltration at Yucca Mountain (Continued)

Input Parameter	Value/Distribution	Basis/Reference
Infiltration rate, *u* [mm/year]	Uniform distribution from 1 to 45	In CRWMS M&O 2000 [DIRS 153246], Table 3.2-2, glacial-transition average infiltrations are given as 2.2 mm/yr for low (probability 17%), 20 mm/yr for medium (probability 48%), 37 mm/yr for high (probability 35%). The weighted average infiltration is then approximately 23 mm/yr (0.17x2.2 + 0.48x20 + 0.35x37). The limits of the uniform distribution are chosen to range from below the low-case mean to above the high-case mean, with the appropriate weighted mean of 23 mm/yr. A nice, simple choice is a uniform distribution from 1 to 45 mm/yr.

Table 4.3.5-4. Summary of Uncertainty Issues Related to Thermohydrologic Effects on Seepage

Category	Uncertainty Issue	Treatment of Uncertainty Issue	Affected Goals
Parameter uncertainties	Thermal operating modes	Sensitivity studies for both higher- and lower-temperature operating modes	Thermal effects on UZ flow and seepage
	Impact of lithophysal cavities on thermal properties	Incorporate effects of lithophysal cavities in thermal conductivity and heat capacity values Sensitivity studies using properties with and without effects of lithophysal cavities	Temperature distribution, thermal effects on seepage
	Temperature-dependent heat capacity of the rock mass	Needs to be incorporated for sensitivity studies	Temperature distribution, spatial and temporal
	Hydrologic properties	Not expected to be significant for higher-temperature operating mode Need sensitivity studies for lower-temperature operating mode	Seepage
Data uncertainty	Thermal conductivity (effects of lithophysal cavities)	Field measurements needed	Temperature distribution, spatial and temporal
	Effect of faults on thermally induced flow	Sensitivity studies Data limitation, need liquid phase field testing in faults, need characteristic curves in faults	Thermal seepage
Conceptual model uncertainty	Effects of lithophysal cavities on gas and liquid flow	Need new conceptual model and validation against measurements	Redistribution of moisture
	Applicability of "active fracture" option of the dual-permeability model for coupled processes	Need sensitivity studies and validation against planned Cross Drift Thermal Test	Thermal seepage
	Heterogeneity (small scale)	Monte Carlo and sensitivity studies in progress	Thermal seepage
	Ventilation	Only reduction of heat from ventilation has been addressed Need realistic model on moisture removal	Thermal seepage, temperature

Table 4.3.5-4. Summary of Uncertainty Issues Related to Thermohydrologic Effects on Seepage (Continued)

Category	Uncertainty Issue	Treatment of Uncertainty Issue	Affected Goals
Numerical model uncertainty	Assumed geometry of a square drift	Less diversion of water than actual drift geometry	Thermal seepage, shedding of water
	Implementation of capillary barrier within the drift	Different treatment used	Thermal seepage, shedding of water
	Discretization	Different refinement of grids have been implemented Further refinement needed	Temperature, thermal seepage

Table 4.3.6-1. Comparison of Experimental and Potential Yucca Mountain Repository Conditions

	Experimental Conditions	Potential Yucca Mountain System
Thermal gradient	158°C/m	0.75°C/m (BSC 2001 [DIRS 154677], Figure 37b, p. 1126)
Fracture fluid flux	6E-4 m/s	3 E-8 m/s (Bodvarsson 2001 [DIRS 154669], Attachment 4, pp. 37 to 38)
Fracture aperture	31 μm	About 10 to 1,000 μm (small-scale fracture aperture measurements to 200μm were observed as reported in DTN: GS990908314224.009 [DIRS 146877]; smaller scale apertures inferred from modeling results)

Source: Experimental conditions DTN: LB0101THCPRCPX.001 [DIRS 154577].

Table 4.3.6-2. Summary of Uncertainty Issues Related to the Prediction of Thermal-Hydrologic-Chemical Effects on Seepage and Potential Seepage Chemistry

Category	Uncertainty Issue	Treatment of Uncertainty Issue	Affected Goals
Conceptual Uncertainties	Uncertainty in the dual-permeability model and its extension for coupled THC processes	Has not been treated directly Treated indirectly through model validation with the Drift Scale Test	Cannot resolve changes in matrix hydrologic properties and geochemistry near the fracture wall and effects on imbibition
	Mineral precipitation and dissolution take place nonuniformly in the fracture medium and in the matrix	Not treated directly, but indirectly as follows: In initial report, implemented an active fracture model that limits the reactive surface area and the area for diffusive transport between fractures and matrix In update, implemented permeability relation to change in hydraulic aperture, which captures the effect of mineral precipitation in narrower apertures Treated indirectly through model validation	Leads to uncertainty in the range of predicted changes in hydrologic properties and flow

Table 4.3.6-2. Summary of Uncertainty Issues Related to the Prediction of Thermal-Hydrologic-Chemical Effects on Seepage and Potential Seepage Chemistry (Continued)

Category	Uncertainty Issue	Treatment of Uncertainty Issue	Affected Goals
Conceptual Uncertainties	Effect of lithophysae on THC processes	Effect on thermal properties treated in post-update analyses Effect on hydrologic properties and their effect on transport and coupled THC processes were not treated	Results in greater uncertainty in the width of boiling zone and associated zone of maximum mineral precipitation. Adds uncertainty to gas phase transport and timing of simulated gaseous carbon dioxide concentrations
	Changes in infiltrating water chemistry and associated climate changes	Assessed indirectly through simulations using alternate water compositions	Results in more uncertainty in the range of potential chemical compositions during post-thermal period
	Implementation of THC numerical approaches in transitions from boiling to dryout zones	Reduced minimum liquid saturation for treating chemical reactions and refined to capture saturation gradients Assessed effect in extreme case of steep thermal gradient and narrow zone of saturation decline to zero	Adds uncertainty to prediction of maximum changes in hydrologic properties and transient changes in water chemistry during dryout and rewetting at a subgrid scale
Data Uncertainties	Composition of fracture water	Post-update analysis used alternative perched water analysis for fracture, matrix, and infiltrating water composition	Not a significant factor during early thermal period, but adds to uncertainty during port-thermal period as percolating waters rewet the drift
	Matrix pore water compositions	Alternate pore water analyses used in post-update analyses	Limits the range of potential water compositions that are predicted
	Thermodynamic and kinetic data	Treated through sensitivity studies on long-term behavior of ambient system chemistry, assuming a fixed infiltration rate Many uncertainties unknown and treated through model validation (Drift Scale Test and laboratory experiments)	Adds uncertainty to ranges of predicted water compositions, mineral assemblages, and changes in hydrologic properties
Parameter Uncertainties	Range in fracture porosity	Not treated directly Effect on permeability treated indirectly through implementation of permeability relation to hydraulic aperture	Limits range of possible effects on hydrologic properties and transport
	Heterogeneity	Fracture permeability treated heterogeneity in updated report Heterogeneity in matrix properties not treated Local heterogeneity in mineralogical properties not treated Heterogeneity in initial water geochemistry not treated directly; treated indirectly through alternate compositions	Matrix properties not significant because of low permeability Heterogeneity in mineralogic properties could amplify local effects on hydrologic properties Heterogeneity in water chemistry could lead to local mixing effects, leading to a greater range in uncertainty in predicted chemistry

Table 4.3.6-2. Summary of Uncertainty Issues Related to the Prediction of Thermal-Hydrologic-Chemical Effects on Seepage and Potential Seepage Chemistry (Continued)

Category	Uncertainty Issue	Treatment of Uncertainty Issue	Affected Goals
Parameter Uncertainties	Uncertainty propagation	Deterministic seepage chemistry and effects on seepage (i.e., flow) predictions over limited range of potential parameter values Distribution of other input parameters (e.g., infiltration and heat loading) developed based on deterministic runs and sensitivity analyses.	Distribution of parameters in TSPA calculation

Table 4.3.7-1. Input Parameters and Data Tracking Numbers for Distinct Element Analysis

Description	Value	Units	Data Tracking Number
Matrix Properties			
Dry Bulk Density	2,270	kg/m^3	MO0003SEPDRDDA.000 [DIRS 147607]
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	degree	MO0003SEPDRDDA.000 [DIRS 147607]
Joint Cohesion	0.09	MPa	MO9911SEPGRP34.000 [DIRS 148524]
Joint Dilation Angle	29	degree	MO9911SEPGRP34.000 [DIRS 148524]
Initial Joint Aperture	0.098	mm	LB990501233129.001 [DIRS 106787]
Thermal Properties			
Thermal Expansion Coefficient	9.73E-6	degree C^{-1}	MO0004RIB00035.001 [DIRS 153848]
Stress and Stress Gradient			
In Situ Stress	7.6	MPa	MO0007RIB00077.000 [DIRS 154087]
Vertical Stress Gradient	0.023	MPa/m	MO0007RIB00077.000 [DIRS 154087]
Input Temperatures			
Input Temperatures	various	degree C	LL000114004242.090 [DIRS 142884]

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

Table 4.3.7-2. Permeability Ratio Distribution for Horizontal Fractures

Time (years)	Permeability Ratio (%)							
	1.00E-5	1.00E-3	0.01	1	10	100	1000	Total
10	3.6	0.8	16.8	59.9	12.0	3.3	3.7	100
50	1.1	0.3	2.6	67.0	21.6	3.5	3.9	100
55	4.4	0.6	16.0	59.2	12.2	2.9	4.8	100
100	2.2	0.3	3.4	62.4	23.6	3.1	5.0	100
200	1.5	0.1	0.9	43.3	44.3	4.2	5.7	100
400	1.4	0.1	0.8	50.9	36.7	4.4	5.7	100
1000	1.5	0.1	0.8	55.2	32.2	4.6	5.7	100
100,000	0	0	0	2.2	45.5	40.9	11.4	100

Source: Blair 2001 [DIRS 155005], Table 4.

Table 4.3.7-3. Permeability Ratio Distribution for Vertical Fractures

Time (years)	Permeability Ratio (%)							
	1.00E-5	1.00E-3	0.01	1	10	100	1000	Total
10	4.7	2.7	43.2	40.2	4.7	2.1	2.4	100
50	3.1	2.1	49.6	35.6	5.0	2.2	2.5	100
55	62.6	7.6	17.6	5.6	2.0	1.8	2.7	100
100	80.6	2.8	7.3	3.0	1.81	1.7	2.8	100
200	75.7	4.0	9.3	3.9	2.3	1.9	3.0	100
400	74.2	4.0	10.2	4.2	2.5	2.0	3.0	100
1000	69.9	5.1	12.3	4.9	2.7	2.0	3.1	100
100,000	0	0	0	3.9	18.6	61.8	15.7	100

Source: Blair 2001 [DIRS 155005], Table 5.

Table 4.3.7-4. Thermal-Hydrologic-Mechanical Property Parameters Used in Simulations

Parameter	Tptpmn	Tptpll	Source
Young's modulus	14.77 GPa	14.77 GPa	CRWMS M&O 1999 [DIRS 126475], Table 10 to 15 and Table 24
Poisson's ratio	0.21	0.21	
Cohesion	2.6 MPa	2.6 MPa	
Friction angle (degrees)	57	57	
Dilation angle (degrees)	29	29	
Thermal expansion coefficient	4.14 E-6 /°C	4.14 E-6 /°C	
Tensile strength	1.54 MPa	1.54 MPa	
Initial hydraulic aperture for Equation 4.3.7-2, b_i	80.0 μm	164.8 μm	The value of b_i is calculated from mean fracture spacing (s) and isotropic permeability assuming an ideal cubic block model, leading to the following formula: $b_i = \sqrt[3]{k \times 6 \times s}$ (Bodvarsson 2001 [DIRS 154669], Attachment 9, pp. 21 to 29)
Maximum joint closure for Equation 4.3.7-2, b_{max}	541.6 μm	541.6 μm	Determined by model calibration against air-permeability experiments at ESF niches and Drift Scale Test (Bodvarsson 2001 [DIRS 154669], Attachment 9, pp. 12 to 26)

Table 4.3.7-4. Thermal-Hydrologic-Mechanical Property Parameters Used in Simulations (Continued)

Parameter	Tptpmn	Tptpll	Source
Exponent for Equation 4.3.7-2, α (1/Pa)	1.1 E-6	1.1 E-6	Determined by model calibration against air-permeability experiments at ESF niches and Drift Scale Test (Bodvarsson 2001 [DIRS 154669], Attachment 9, pp. 12 to 26)
Gradient of vertical stress σ_v	0.022 MPa/m	0.022 MPa/m	Within range of field measurements by Stock et al. (1985 [DIRS 101027]) and Lee and Haimson (1999 [DIRS 129667])
Horizontal stress σ_h	$0.35 \times \sigma_v$ MPa	$0.35 \times \sigma_v$ MPa	

Table 4.3.7-5. Summary of Uncertainty Issues Related to Thermal-Hydrologic-Mechanical Effects on Seepage

Category	Uncertainty Issue	Treatment of Uncertainty Issue	Affected Goals
Conceptual Model Uncertainties	Use of two-way coupling versus fully coupled THM coupling	TM analysis and fully coupled THM analyses have been done (Section 4.3.7.4.4)	Flux around drift and seepage into drift
	Use of distinct element method versus continua method	Distinct element and continua methods have been used (Sections 4.3.7.3 and 4.3.7.4) Reconciliation of the outcomes of the two methods to be conducted	Flux around drift and seepage into drift
	Capillary-permeability relationship	Leverett's relationship was used (Section 4.3.7.4.2); sensitivity studies to be conducted	Flux around drift and seepage into drift
Model Geometry Uncertainties	Boundary conditions used	A reasonable choice of boundary conditions was made for the current studies. Sensitivity study with range of conditions to be conducted	Flux around the drift and seepage into drift
	Drift near edge of repository	Current study considers a drift away from the repository boundary. Simulation of a drift near edge of repository to be conducted	Flux around the drift and seepage into drift
Parameter Uncertainties	Rock fracture stiffness in the layers Residue permeability values	Current values used were obtained from a calibration study using the ESF niche and Drift Scale Test data (Section 4.3.7.4.3) A complete THM analysis of the Drift Scale Test with supplementary measurements to be conducted	Change in permeability around seepage into drift
	Heterogeneity in permeability spatial distribution	Current study uses multiple hydrostratigraphic layers vertically; however, it assumes homogeneous properties within each layer. Additional simulations needed on heterogeneous field representing the hydrogeologic units. Studies with multiple realizations to be conducted	Flux around the drift and seepage into drift

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