Table 4-16. Thermal-Hydrologic Variables Predicted with the Multiscale Thermal- Hydrologic Model at 610 Locations in the Potential Repository

Thermal-Hydrologic Variable	Drift-Scale Location at Which Predicted
Temperature	Near-field environment host rock (5 m [16 ft] above crown)
	Near-field environment host rock (mid-pillar at potential repository horizon)
	Maximum lateral extent of boiling
	Upper drift wall (crown of the drift)
	Lower drift wall (below invert)
	Drift wall (perimeter average)
	Drip shield (perimeter average)
	Drip shield (upper surface)
	Waste package (surface average)
	Invert (average)
Relative humidity	Drift wall (perimeter average)
	Drip shield (perimeter average)
	Waste package
	Invert (average)
Liquid saturation (matrix)	Drift wall (perimeter average)
	Drip shield (perimeter average)
	Invert
Liquid-phase flux	Near-field environment host rock (5 m [16 ft] above crown)
	Near-field environment host rock (3 m [10 ft] above crown)
	Drift wall (crown)
	Drip shield (crown)
	Drip shield (upper surface average)
	Drip shield (lower side at the base)
	Invert (average)
Gas-phase air-mass fracture	Drip shield (perimeter average)
Gas-phase pressure	Drip shield (perimeter average)
Capillary pressure	Drip shield (perimeter average)
	Invert (average)
	Drift wall (crown; in matrix)
	Drift wall (crown; in fractures)
Gas-phase (water vapor) flux	Drift wall (perimeter average)
Gas-phase (air) flux	Drift wall (perimeter average)
Evaporation rate	Drip shield (crown)
	Drip shield (perimeter total)
	Invert (total)

are run for 31 locations spaced throughout the potential repository area (Figure 4-65) for a range of thermal loading values that represents the influence of edge-cooling. Variability of the hydrologic properties at the scale of the potential repository is represented by the 31 locations (CRWMS M&O 2000cf, Section 5.1.1).

The other three types of models, which are thermal conduction-only models, are required to account for the influence of three-dimensional mountain-scale heat flow and three-dimensional drift-scale heat flow on drift-scale thermal-hydrologic behavior. Further details on these thermal-conduction-only models, the method used to modify the two-dimensional thermal-hydrologic model results to reflect the three-dimensional scale effects, and the representation of air spaces in the drifts are provided in supporting documentation (CRWMS M&O 2000cf, Sections 6 and 7.1).

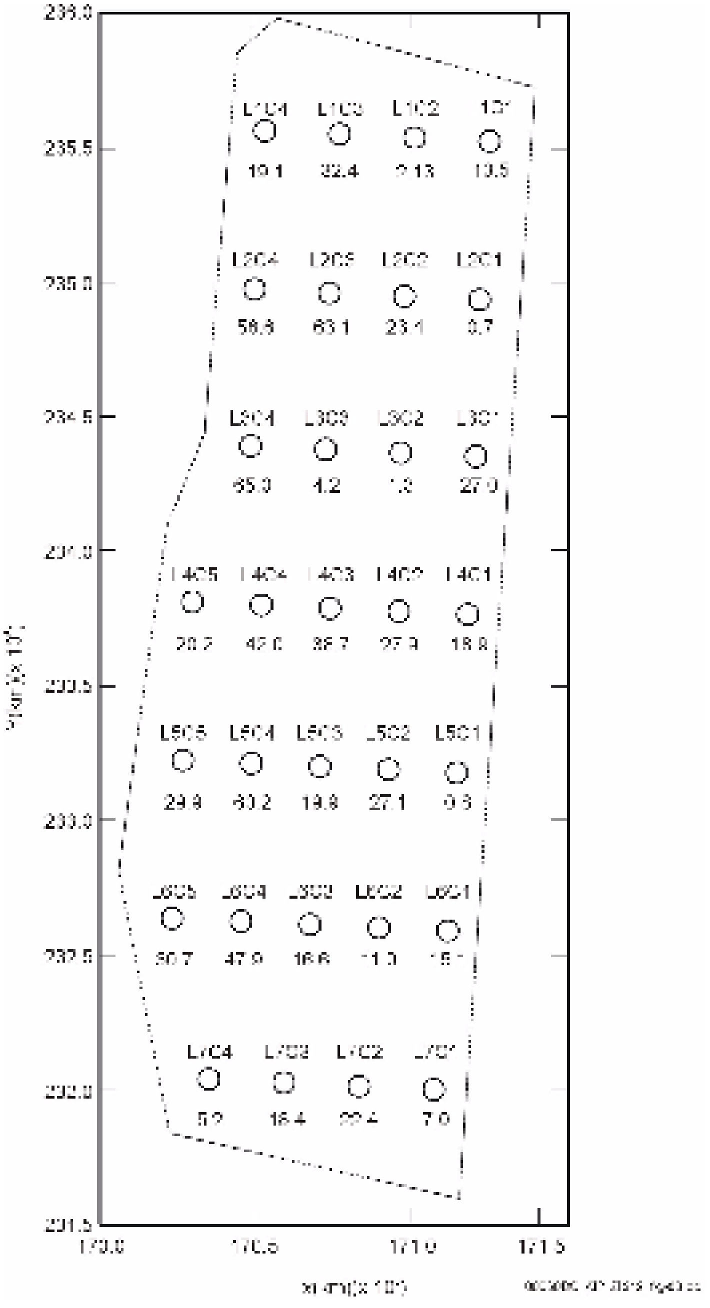

Figure 4-65. Layout of the Potential Repository Used in the Multiscale Thermal-Hydrologic Model
These 31 locations (labeled L1C1 through L7C4) represent the overall repository in the multiscale thermal-hydrologic model. Detailed modeling is performed for each location to predict temperature and humidity conditions in the emplacement drifts. These models are combined with larger (but coarser) drift-scale and mountain-scale models to incorporate the effects of large-scale features of the site and the repository layout. The values posted at each location are the net infiltration values for the glacial-transition (long-term) climate state. Source: CRWMS M&O 2000as, Figure 3-70.

In the multiscale thermal-hydrologic model, the waste package sequence is explicitly modeled in a drift segment and repeated hundreds of times throughout the footprint of the potential repository. Model geometry is consistent with the design basis described in this report. The emplaced waste packages fall into several categories, representing those that would contain (1) pressurized water reactor spent nuclear fuel, (2) boiling water reactor spent nuclear fuel, (3) DOE high-level radioactive waste, and (4) DOE (naval) spent nuclear fuel. All waste packages are emplaced at the same time and follow the same average thermal decay function (as a percentage of initial heat output). The 70 percent heat-removal efficiency and the 50-year ventilation period are applied uniformly throughout the potential repository footprint. The overall average areal mass loading of the potential repository for multiscale model applications is 60 MTHM/acre.

Figure 4-65 illustrates the potential repository footprint used in the model; this footprint closely approximates the actual plan view of the perimeter within which waste would be emplaced. Thirty-one locations are shown, which represent the lateral variability in hydrologic properties, stratigraphic thickness, and boundary conditions.

Major results of the multiscale thermal-hydrologic model summarized in this section are based on the higher-temperature thermal operating mode described in Section 2. During the preclosure period, host rock temperatures remain below the boiling point for the mean- and upper-infiltration flux cases, while boiling occurs in the host rock for the lower-flux case.

The expected duration of temperatures above the boiling point of water (96°C [205°F]) on the surfaces of the waste packages varies for three main reasons: (1) location within the repository layout, (2) spatial variation in the infiltration of recharge water at the ground surface, and (3) variability in the heat output of individual waste packages. The repository edges would cool first because they lose heat to the cooler rock outside the layout. The repository center would cool more slowly because heat flow would be limited mainly to the upward and downward directions. Water percolating downward through the host rock in response to infiltration at the ground surface would hasten cooling of the repository; locations with greater percolation will cool sooner. There will be relatively large variations in the heat output of individual waste packages depending on the type and age of the waste they contain. Each of these effects is represented explicitly in the multiscale thermal-hydrologic model, and the results of this model are used in TSPA.

During the preclosure period, peak waste package temperatures of 100°C (212°F) for the mean flux case, and 110°C (230°F) for the low flux case, are expected to occur at 10 to 15 years; peak drift-wall temperatures of 86°C (187°F) for the mean flux case, and 96°C (205°F) for the low flux case, are expected to occur at 20 to 25 years. Edge-cooling effects will not strongly affect preclosure temperatures.

During the postclosure period, peak waste package temperatures of 128° to 178°C (262° to 352°F) for the mean flux case, 127° to 189°C (261° to 372°F) for the low flux case, and 124° to 173°C (255° to 343°F) for the high flux case are expected to occur at 60 years. The difference in peak waste package temperature between the hottest and coldest waste packages for the mean flux case would be approximately 50 C° (90 F°). During the very early postclosure period, edge-cooling will have a small effect on temperatures. By 100 years, the influence of edge-cooling will be considerable, with waste package temperatures varying by 65 C° (117 F°) (98° to 163°C [208° to 325°F]) from the edge to the center of the potential repository for the mean flux case.

A typical waste package under nominal conditions would have an average surface temperature above the boiling point of water for about 1,000 years (CRWMS M&O 2000cf, Figure 6-50). For the mean infiltration case, the average temperature on the surfaces of all 21-PWR waste packages would cool to below the boiling point of water after about 1,400 years. Lower infiltration rates could increase the time until the waste packages cool to this temperature. Depending on the infiltration rate and the location in the repository, the time to cool could be less; for example, for the mean infiltration rate a 21-PWR waste package located on the edge of the repository would cool to below the boiling temperature of water within about 300 years. For brevity, these ranges are described elsewhere in this report as "from hundreds to thousands of years."

Liquid-phase flux in the host rock above the drift would be influenced by dryout and heat pipe activity. Heat pipe behavior can increase the liquid-phase flux in fractures to well above the ambient percolation flux. However, the duration of this effect would be greatly decreased in this design in comparison with the repository design used for the Viability Assessment (CRWMS M&O 1998g, Chapter 3, Section 3.5.4). For the higher-temperature operating mode, the increased liquid-phase flux is calculated to last for less than 600 years (the duration of the present-day climate period).

The maximum lateral extent of boiling temperatures (away from the drift wall) is a good indication of spatial extent of dryout around the emplacement drifts. The lateral extent of boiling would be greater for the low infiltration-flux case than for the mean or upper-flux cases. For the hottest waste package location and the lower flux distribution, the maximum lateral extent of boiling would be 18 m (59 ft); because the drifts would be 81 m (266 ft) apart, a maximum of approximately 44 percent of the potential repository area would exceed the boiling point. If the estimated infiltration increases, this percentage would decrease.

There is a much greater difference in dryout behavior (as evidenced by the maximum lateral extent of boiling and by relative humidity reduction) between the mean and low infiltration-flux cases than between the mean and upper flux cases. Therefore, if one considers a percolation threshold above which rock dryout becomes substantially limited by percolation, the threshold would be near the mean infiltration-flux case. Larger values of the percolation flux greatly limit the calculated extent of boiling temperatures and rock dryout.

4.2.2.3.3 Drift-Scale Thermal-Hydrologic-Chemical Processes and Models

Figure 4-40 shows schematically the relationships between thermal-hydrologic and geochemical processes in the zones of boiling, condensation, and water drainage in the rock surrounding the potential repository, particularly in the rock above the emplacement drifts. The emphasis in this section is on the changes in flow properties of the host rock due to these processes. Modeling of thermal-hydrologic-chemical effects on the aqueous chemistry of seepage water and gas composition in the potential repository host rock is described in Section 4.2.3.3.

Changes to hydrologic properties were evaluated using the thermal-hydrologic-chemical model. The thermal-hydrologic-chemical models account for two-dimensional heat and mass transfer within the drifts and in the surrounding rock, using separate continua in the rock to represent the connected network of fractures and the rock matrix in which the fractures reside (CRWMS M&O 2000al, Section 3.2.3.4.2). The thermal-chemical model component is implemented using TOUGHREACT, a heat transfer, mass transfer, and reactive-transport code. The model is used to calculate dissolution and precipitation of minerals that could change the porosity and permeability of the fracture system (CRWMS M&O 2000al, Section 3.2.3.4.3).

Thermal-hydrologic aspects of the model, such as the heating rate, ventilation, infiltration flux, and other boundary conditions, are identical to the thermal-hydrologic models discussed previously in this section. Discretization of the model domain is illustrated in Figure 4-66. Several cases were evaluated for different infiltration conditions (i.e., lower, mean, and upper) using the same climate-change scenarios used for the unsaturated zone flow model (BSC 2001o, Section 6.3).

The dual-permeability method was selected for modeling thermal-hydrologic-chemical processes. This is an important selection because a realistic representation of chemical interactions between fractures and the rock matrix depends on realistic representation of hydrologic interactions. The active fracture model is used (Liu et al. 1998; CRWMS M&O 2000bq, Section 6.4.5). Each matrix gridblock and each fracture gridblock has its own pressure, temperature, liquid saturation, water and gas chemistry, and mineralogy. Water–mineral reactions are considered to take place

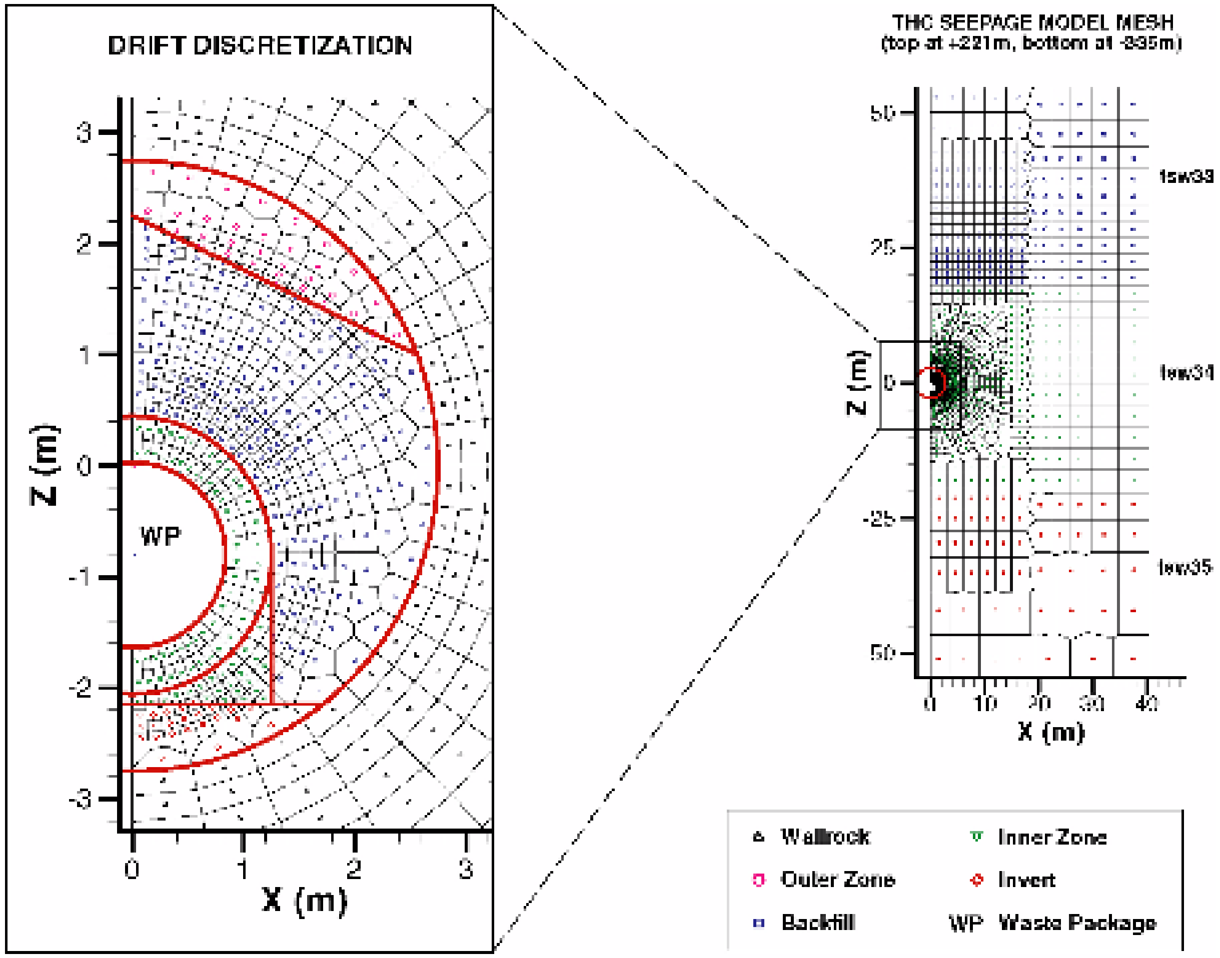

Figure 4-66. Thermal-Hydrologic-Chemical Seepage Model Mesh Showing Hydrogeologic Units in Proximity of the Drift, and Blowup Showing Discretization of In-Drift Design Components

The hydrogeologic units shown are the Topopah Spring Tuff upper lithophysal (tsw33), middle nonlithophysal (tsw34), and lower lithophysal (tsw35) units. These model grids are for simulations with backfill. The model results are used to predict thermal, hydrologic, and chemical conditions at the drift wall, rather than inside the drift. The results are therefore considered applicable to the design without backfill. THC = thermal-hydrologic-chemical. Source: CRWMS M&O 2000c, Figure 3.10-6.

under either kinetic or equilibrium conditions, using simulation methods similar to those described by Reed (1982) and Steefel and Lasaga (1994). Because the dissolution rates of many mineral–water reactions are quite slow, most phases are treated using pseudo-order reaction kinetics.

As stated in Section 4.2.2.2.1.3, the initial water and gas chemistry selected for use in the thermal-hydrologic-chemical model is based on the chemical composition of matrix pore water collected from Alcove 5 (BSC 2001o, Sections 4.1.3 and 6.1.2). Although the rock permeability of the matrix is many orders of magnitude smaller in the matrix than in the fractures, the TSPA-SR thermal-hydrologic-chemical model assumes that infiltrating water in the fractures has the same composition as matrix pore water. This is justified in that the chloride-sulfate-type matrix-derived pore water composition is more concentrated in total dissolved minerals. The actual water composition within fractures tends to be more dilute (i.e., bicarbonate-type water). For all thermal-hydrologic-chemical modeling, the initial water composition is set to be the same in the fractures and matrix throughout the model domain (BSC 2001o, Section 4.1.3). Thermal-hydrologic-chemical model simulations were repeated with two sets of rock minerals to evaluate the sensitivity of calculated results to the mineral assemblage selected (BSC 2001o, Section 6.2). A full-simulation case included the major minerals found in the fractures and matrix of all rock units that are likely to be thermally perturbed based on mineral occurrence in deeper zeolitized units. A limited-simulation case included those minerals needed to represent basic aspects of Drift Scale Test data, such as pH and gas-phase carbon dioxide, while neglecting other species, such as silicates, ferric minerals, and fluorides. Details on derivation of model inputs, the numerical model and supporting sensitivity studies are provided in *Drift-Scale Coupled Processes (DST and THC Seepage) Models* (BSC 2001o, Sections 4.1 and 6.2).

Thermal-hydrologic-chemical model results consist of projections for the composition of water and gas that may enter the emplacement drifts for 100,000 years, including a 50-year preclosure period with ventilation. Figure 4-67 shows liquid saturation and temperature in the rock around the drifts at 600 years for the three infiltration conditions (i.e., lower, mean, and upper). This is the approximate time of the maximum extent of dryout for each infiltration case investigated. Note that these models predict conditions that would be encountered near the center of the potential repository, and that cooler conditions would be found near the edges.

Time histories for gas-phase carbon dioxide concentration, pH, chloride concentration, and total dissolved carbon concentration are predicted for the several locations in the host rock at the drift wall (CRWMS M&O 2000c, Figures 3.10-8 to 3.10-11). These results are summarized in Section 4.2.3.3, where they are used as boundary conditions for the physical and chemical environment in the emplacement drifts.

Comparison with data from the Drift Scale Test shows that the limited simulation (calcite, silica, and gypsum minerals only) matches observed chemical data more closely than the full simulation (including silicates, iron, and fluorides). However, for longer duration of reflux and boiling, as would be encountered in the potential repository, the system may trend toward the chemistry of the more complex full simulation.

Porosity changes in the rock matrix and fractures are directly related to volume changes from mineral precipitation and dissolution. Changes in fracture permeability are approximated using a parallel-plate model approach with fractures of uniform aperture (Steefel and Lasaga 1994, p. 556). Matrix permeability changes are calculated from changes in porosity using the Carmen–Kozeny relation (Bear 1988, p. 134). Capillary pressure in the matrix and fractures is modified using the Leverett scaling relation (Slider 1976, pp. 290 to 297), as previously mentioned in Section 4.2.1.3.2.

The calculated changes in fracture porosity for rock near the emplacement drifts, for the full simulation, at a simulation time of 10,000 years, are shown in Figure 4-68 for the three infiltration conditions (i.e., lower, mean, and upper). The fracture porosity change is expressed as a percentage of the initial porosity. Maximum porosity decrease is predicted for the high-infiltration case, predominantly above the drift. For all cases, the porosity change is relatively small (less than 1 percent of the initial porosity). For the limited simulation, porosity decrease results mainly from calcite precipitation, as was interpreted from the Drift Scale Test simulations. For the full simulation, the fracture porosity change is dominated by zeolite reactions. Because the fracture porosity changes are small compared to total fracture porosity, permeability changes are negligible and thermal-hydrologic processes will not be significantly affected by mineral precipitation or dissolution (CRWMS M&O 2000al, Section 3.2.3.4.3).

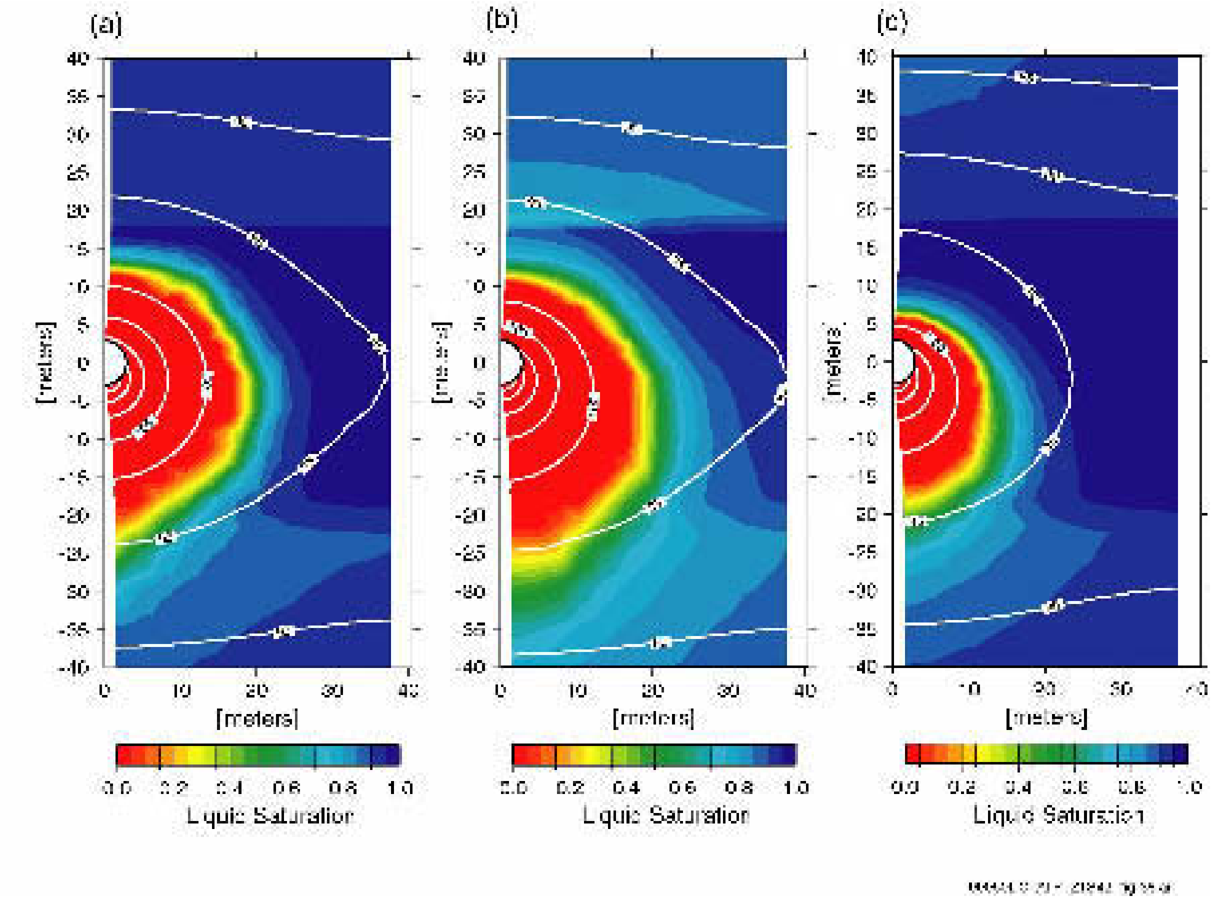

Figure 4-67. Contour Plot of Modeled Liquid Saturations and Temperatures in the Matrix at 600 Years (Near Maximum Dryout) for Three Infiltration Rate Scenarios

The lower, mean, and upper infiltration rate scenarios are developed for the unsaturated zone flow model to represent the uncertainty of present-day and predicted future infiltration rates. The contour plots shown are (a) lower, (b) mean, and (c) upper scenarios (calcite-silica-gypsum system). The white contour lines show temperature in °C. The white half-circle in each plot is the drift outline, and the models are laterally symmetrical about the drift center. Source: CRWMS M&O 2000c, Figure 3.10-7.

4.2.2.3.4 Drift-Scale Thermal-Hydrologic-Mechanical Processes and Models

The drift-scale thermal-hydrologic-mechanical modeling in support of the TSPA accomplishes two objectives. This section emphasizes the potential effect on hydrologic properties in the surrounding rock resulting from thermal-mechanical changes, specifically potential effects on permeability. The drift degradation analysis presented in Section 4.2.3.3.5 assesses thermally caused movement of blocks on fractures intersecting the drift and the potential for rockfall to affect the engineered barrier system.

Most prior thermal-mechanical modeling had the objective of determining the evolution of stresses in the near-field rock, in order to estimate the requirements for rock support in the emplacement drifts. These models treated the rock as a continuum and conservatively assumed that the mid-pillar locations were symmetry boundaries. This assumption is conservative (produces higher calculated stresses) because the overall repository footprint can expand due to the heating. The move-

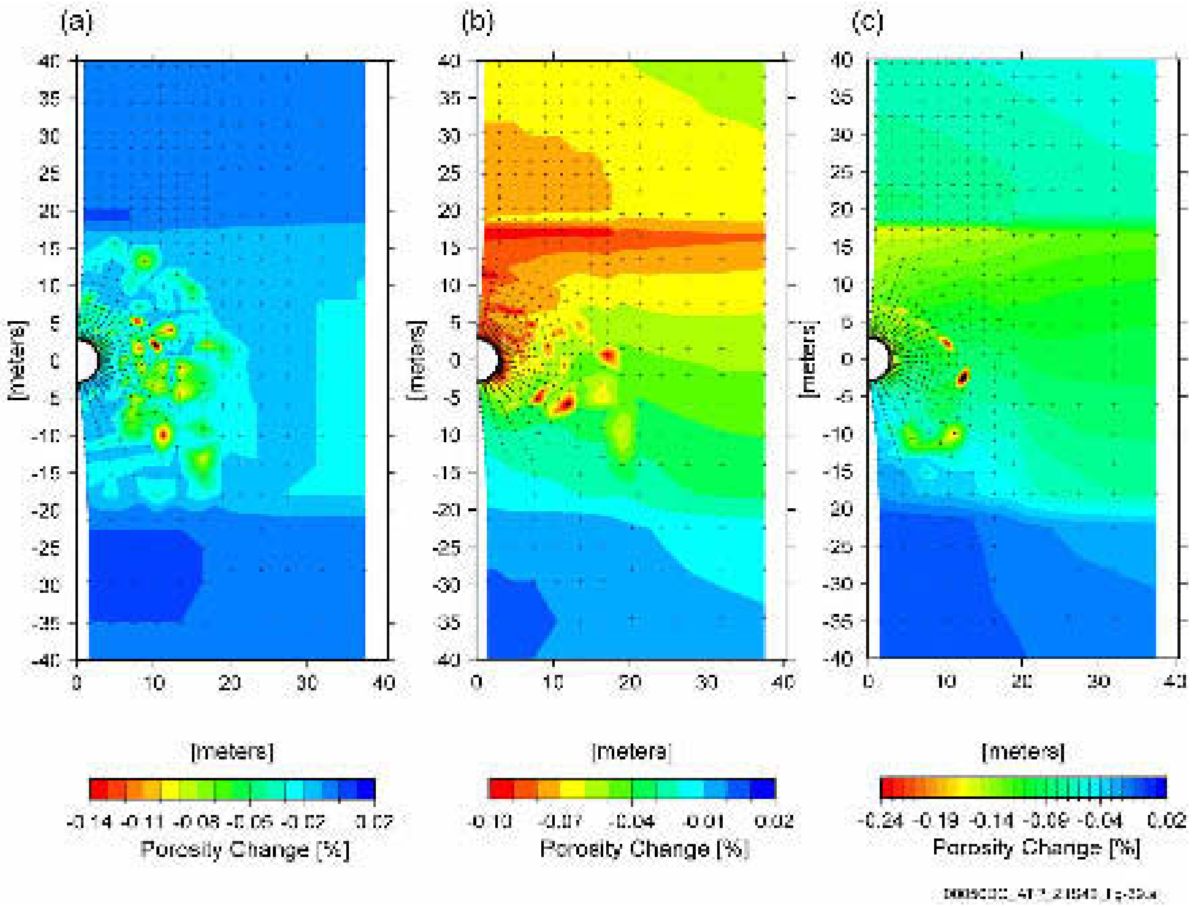

Figure 4-68. Contour Plot of Calculated Total Fracture Porosity Change at 10,000 Years for Three Infiltration Rate Scenarios

The lower, mean, and upper infiltration rate scenarios are developed for the unsaturated zone flow model to represent the uncertainty of present-day and predicted future infiltration rates. The contour plots shown are (a) lower, (b) mean, and (c) upper scenarios (full simulation). Red areas indicate the maximum decrease in porosity as a result of mineral precipitation. The white half-circle in each plot is the drift outline, and the models are laterally symmetrical about the drift center. Source: CRWMS M&O 2000c, Figure 3.10-12.

ment of rock blocks at fractures was captured in the continuum models by the rock mass properties, such as the coefficient of thermal expansion (the fractional expansion of the rock per degree of temperature rise). Measurements of this coefficient depends on the size of the sample, with the coefficient decreasing as the scale moves from core to small blocks to small field tests and then to large field tests (CRWMS M&O 1999m, Table 9-3). The decrease in expansion coefficient can be attributed to the increased number of fractures which can accommodate expansion of the rock blocks. The results of the modeling indicate that horizontal compressive stresses increase more than vertical compressive stresses during the thermal pulse, due to the stiff boundary conditions at the mid-pillar locations.

In this analysis supporting the TSPA-SR model, the distinct-element code 3DEC is used to simulate normal and shear displacement and other behavior on discrete fractures in the rock mass surrounding the drift (CRWMS M&O 2000al, Section 3.5.2). Fracture orientations and fracture densities are represented and discretized (gridded) in three dimensions. Fracture orientations are based on field observations (Albin et al. 1997). Joint and rock-mass properties used in the calculation are based on field and laboratory studies of rock and fracture behavior, such as those by Barton et al. (1985) and Olsson and Brown (1994). Fracture densities are based on the assumption that only a few well-connected fractures are mechanically and hydrologically active (CRWMS M&O 2000al, Section 3.5.2).

Calculated joint deformations are used to compute permeability deformation values over a period of 1,000 years to capture the effects of heating and cooling. The mathematical formulation is described in the *Near-Field Environment Process Model Report* (CRWMS M&O 2000al, Section 3.5.2.3). Using this formulation, shear deformation always produces an increase in permeability, while normal deformation will increase permeability if the fracture opens and decrease permeability if the fracture closes. In general, fracture closing is expected during the heating phase in response to thermal expansion, while fracture opening occurs during cooling, the effects of shear displacements notwithstanding.

The results of the calculation (CRWMS M&O 2000al, Section 3.5) are that the major thermal-mechanical effect on fracture permeability occurs during cooldown due to both shear and normal deformation. Shear deformation of fractures during the cooldown causes permeability of the fractures in a region within two drift diameters of a drift wall to increase in permeability as much as an order of magnitude. Specifically, shear deformation on vertical fractures during cooldown produces the maximum amount of permeability change. Farther away from the drift wall, smaller increases in permeability (a factor of five) may occur on vertical fractures (CRWMS M&O 2000al, Section 3.5.3).

Results also indicate that normal deformation of fractures causes permeability to increase but to a lesser degree than shear deformation. Normal deformation during heating causes permeability to decrease significantly within one drift diameter of the drift wall. During cooldown, some vertical fractures above the drift open, thus increasing the permeability by a factor of two from the ambient values (CRWMS M&O 2000al, Section 3.5.3).

Ambient fracture permeability at the repository horizon is high, greater than 10^{-13} m^2 (100 millidarcy) (CRWMS M&O 2000ch, Table 5). *Near-Field Environment Process Model Report* (CRWMS M&O 2000al, Section 5.5) concludes that the potential order of magnitude increase in permeability due to shear movement is not likely to significantly affect seepage.

4.2.2.3.5 Limitations and Uncertainties

As discussed in Section 4.1.1.2, uncertainties are an inherent component of the TSPA method. Uncertainty is introduced through the conceptual model selected to characterize a process, as well as the mathematical, numerical, and computational approaches used to implement the model. Uncertainty is also introduced from imperfect knowledge of important parameters used for input to the models (e.g., physical properties).

The DOE has performed several supplemental activities to address uncertainties and limitations in the TSPA-SR model. Additionally, as noted in Section 4.1.4, the DOE is evaluating the possibility for mitigating uncertainties in modeling long-term repository performance by operating the design described in this report at lower temperatures. Consequently, some of the models describing the effect of decay heat on water movement have been updated since the TSPA-SR model. Some alternative conceptual models have been implemented, and sensitivity analyses conducted to address parameter and model uncertainties. These supplemental model analyses are summarized in *FY01 Supplemental Science and Performance Analyses* (BSC 2001a, Section 1; BSC 2001b, Section 1).

Mountain-Scale Thermal-Hydrologic Model—The unsaturated zone flow model is the basis for the mountain-scale thermal-hydrologic model. Therefore, uncertainties associated with the unsaturated zone flow model also pertain to the mountain-scale model (see Section 4.2.1.3). The spatial resolution of the numerical mountain-scale thermal-hydrologic model is large enough that it limits the interpretation of calculated temperature, saturation, and fluxes within the emplacement drifts and in the host rock near the drift openings. Consequently, the multiscale thermal-hydrologic model, with a finer spatial scale than the mountain-scale model, is used for these purposes.

Multiscale Thermal-Hydrologic Model—Two categories of model uncertainties are defined for the multiscale thermal-hydrologic model: (1) uncertainties related to thermal-hydrologic modeling and (2) uncertainties related to the multiscale estimation methodology.

The unsaturated zone flow model provides an important basis for the multiscale thermal-hydrologic model. Consequently, uncertainties associated with the flow model are propagated to the multiscale thermal-hydrologic model. Uncertainties related to the special features of the unsaturated zone seepage process model are not incorporated in the TSPA-SR model. As discussed in this section, the TSPA-SR model uses a conservative approach for calculating seepage during the thermal pulse, based on the percolation flux (5 m [16 ft] above the drift openings) and calculated by the multiscale thermal-hydrologic model. Although this is considered to be a conservative approach (leading to overestimated thermal seepage into drift openings), model improvements have been suggested such as discrete representation of flow focusing along faults and fractures and representation of episodically increased flow in the host rock (BSC 2001a, Section 4.3.5.6).

The percolation flux contains uncertainties related to mean, high, and low infiltration flux conditions, temporal variability (e.g., changes in climate), and spatial variability (e.g., repository cooling at the edges). The principal effects of these uncertainties on TSPA are related to the timing for cooling and return of moisture to the in-drift environment. Differences in timing of hundreds to a few thousands of years (as discussed in Section 4.2.2.3.2) will have a minor impact on the estimated longevity of the drip shield and waste package (with expected lifetimes greater than 10,000 years calculated in the TSPA-SR model). Another uncertainty is the arrangement and heat output of different types of waste packages, either in a lower- or higher-temperature operating mode. An arrangement of waste types with different heat output is used in the multiscale model, but the extent to which this is representative of repository conditions is uncertain, pending final decisions on repository design and operations parameters.

Uncertainties related to the multiscale estimation methodology include the effects of mountain-scale gas-phase convective circulation and the movement of water vapor along the axis of emplacement drifts from warmer to cooler regions. The TSPA-SR modeling approach did not include heat transfer by these mechanisms, probably resulting in overestimation of predicted temperatures and the duration of the thermal pulse.

Supplemental studies have added insight to some uncertainties and limitations identified with the TSPA-SR model. Approaches included alternative thermal property sets representing lithophysal tuff, Monte Carlo simulations of spatially heterogeneous fracture properties, simulation of a through-going vertical fracture zone intersecting the drift opening, and decreased thermal loading representing a lower-temperature operating mode (BSC 2001a, Sections 4.3.5.3, 4.3.5.4, and 4.3.5.5). Specific studies included:

- Alternative thermal seepage models incorporating the effects of flow focusing and episodicity (BSC 2001a, Section 4.3.5). The results support previous TSPA-SR analyses that found thermal seepage to be negligible for the relatively small values of seepage that may occur.

- Representation of fractures by spatially heterogeneous properties (BSC 2001a, Section 5.3.1.4.2).

- Evaluation of the bulk permeability of the host rock, the thermal conductivity of the lithophysal Tptpll unit and the invert, and the effects of lithophysal porosity of the Tptpll unit on vapor storage and heat capacity (BSC 2001a, Sections 5.3.1.4.1, 5.3.1.4.7, 5.3.1.4.8, 5.3.1.4.9, and 5.3.1.4.10).

- Evaluation of mountain-scale gas-phase convective process and the movement of vapor along the axis of the emplacement drifts (BSC 2001a, Sections 5.3.1.4.4 and 5.3.2.4.6).

Supplemental studies substantiate the overall model and analytical results of the TSPA-SR model, providing quantification of uncertainty either quantitatively or qualitatively. Thermal-hydrologic-chemical and thermal-hydrologic-mechanical processes will not significantly affect temperature or relative humidity within the emplacement drifts (BSC 2001a, Sections 5.3.1.4.5 and 5.3.1.4.6). In evaluating a lower-temperature operating mode, supplemental studies show thermal perturbations to be less than in the higher-temperature operating mode (BSC 2001b, Sections 3.2.2.6 and 4.2.2).

Drift-Scale Thermal Hydrologic-Chemical Processes Model—Uncertainties exist in the chemical parameters used to describe mineral precipitation and dissolution. Temperatures and flow rates are better constrained than other parameters of these models. Geochemical reactions are strongly influenced by temperature, the presence of water, and mass transport; so while the spatial distribution of mineral precipitation and dissolution is considered to be representative, the quantities minerals formed or dissolved at a given time and location are more uncertain. Furthermore, the potential for rapid boiling in the rock to cause mineral behavior outside the range of the models is recognized.

The assumed initial water and gas compositions as well as the geochemical conceptual model may also introduce uncertainty. Uncertainty is also recognized in the relationship used to determine fracture permeability based on changes in fracture porosity. These model uncertainties affect predictions of host rock pore water chemistry and changes in permeability in the host rock caused by thermal-hydrologic-chemical processes.

Model parameters, such as the effective reaction rates, are calibrated to results from field thermal tests, including the Drift Scale Test. Comparison of model predictions to geochemical data is important for confidence building, and such comparisons have shown that the model is reasonable. Results from the full simulations yield higher pH values than measured in water samples from the Drift Scale Test, which results from a greater calculated reaction rate for feldspars. Therefore, porosity changes as a result of feldspar alteration in the potential repository host rock will probably be slower than predicted, suggesting that the TSPA-SR model gives an upper bound on such changes.

Supplemental studies have added insight to some uncertainties and limitations identified with the TSPA-SR thermal-hydrologic-chemical process and abstractions. These activities included a range of different input data and assumptions, such as host rock mineralogy and thermodynamic input data (BSC 2001a, Sections 4.3.6.3.1 and 6.3.1.6). Studies included:

- Supplemental model validation activities of water and gas compositions conducted for Drift Scale Test results (BSC 2001a, Sections 4.3.6.3.1 and 4.3.6.9)

- Supplemental sensitivity studies of different initial water and gas boundary conditions (BSC 2001a, Section 4.3.6.5)

- Simulated evolution of water and gas compositions in the lower lithophysal as well as the middle nonlithophysal tuff unit (BSC 2001a, Section 6.3.1.4.3).

These additional drift-scale thermal-hydrologic-chemical model simulations support the TSPA-SR evaluation, concluding only negligible changes in fracture permeability resulting from thermal-chemical rock and water interactions (BSC 2001a, Sections 4.3.6.7.4 and 4.3.6.9).

Drift-Scale Thermal-Hydrologic-Mechanical Processes and Models—The thermal-hydrologic-mechanical model, used in the TSPA-SR model, used a simplified thermal history to calculate results (CRWMS M&O 2000al, Section 3.5). Coupling the model to the multiscale thermal-hydrologic model has been suggested as a model improvement. Uncertainties in the TSPA-SR thermal-hydrologic-mechanical model also include mechanical boundary conditions, joint and block properties, block geometry, and the calculation of permeability change due to aperture change.

The model domain for drift-scale near-field thermal-mechanical models is bounded by the mid-pillar locations between the emplacement drifts. For stress calculations, using a zero lateral displacement boundary condition at this location would be conservative (i.e., producing greater horizontal compressive stress) because in reality the entire repository layout can expand, allowing some displacement of the mid-pillar locations during the heating period.

The thermal-hydrologic-mechanical model used in the TSPA-SR model imposed boundary conditions equal to the ambient in situ stress (CRWMS M&O 2000al, Section 3.5). This is nonconservative (producing smaller stresses) because it is equivalent to assuming that more lateral displacement of the repository layout would occur. An alternative method would calculate the overall large-scale repository response in a coarsely gridded model and use the results to develop time-dependent displacement and stress boundary conditions for a drift-scale model. An additional advantage of this method would be the ability to consider the variability of the thermal-hydrologic-mechanical response due to proximity to an edge of the repository.

The joint and rock mass properties are based on field and laboratory studies (CRWMS M&O 2000al, Section 3.5.2). As discussed in Section 4.2.2.3.4, the effective thermal expansion coefficient depends on the size of the sample because of the tendency for fractures to deform in response to thermal stress changes. A similar situation exists for discrete fracture models because the rock between the discretely modeled joint may also include fractures. Also, the input values used for joint friction and cohesion are both variable and uncertain. Possible model improvements include adjusting the model grid for more gradual transitions in block sizes, also using site-specific fracture mapping data to develop the block sizes and shapes.

Supplemental studies have added insight to some uncertainties and limitations identified with the TSPA-SR thermal-hydrologic-mechanical process evaluation. Two models were used to assess selected uncertainties related to thermal-hydrologic-mechanical processes: a revised and extended discrete fracture (distinct element) analysis and a fully coupled thermal-hydrologic-mechanical continuum model (BSC 2001a, Section 4.3.7). These studies evaluated different boundary conceptual models, a simplified cubic-block conceptual model, and alternative empirical nonlinear relationships to calculate permeability change from porosity change (BSC 2001a, Section 4.3.7). Sensitive parameters were identified (e.g., residual permeability and rock stiffness) and conclusions are similar to those reached for the TSPA-SR model: permeability changes are within the range of the ambient seepage model, and thus uncertainty is already captured in the TSPA-SR model (BSC 2001a, Section 4.3.7.5).

4.2.2.3.6 Alternative Conceptual Processes

As with limitations and uncertainties, some of the following alternative conceptual models have been implemented or addressed in supplemental uncertainty analyses. These results are summarized in *FY01 Supplemental Science and Performance Analyses* (BSC 2001a, Section 1; BSC 2001b, Section 1).

Mountain-Scale Thermal-Hydrologic Model and Multiscale Thermal-Hydrologic Model—Alternative conceptual models can be organized in several categories: representation of fractured rock in numerical models, selection of representative property values, the potential for permanent changes in those properties from the effects of heating, and alternative models implemented to quantify uncertainties.

The host rock is represented in the mountain-scale and multiscale models as a continuous porous medium, although the rock contains discontinuities such as fractures and fracture zones. An alternative model represents the fractures discretely, and the resulting discrete fracture model approach has been applied to example problems (Hardin 1998, Section 3.3.3). The approach is very computationally intensive and probably not practical for drift-scale and mountain-scale calculations. In addition, the number of interconnected fractures present in the host rock is so large that features of the network can be represented by a continuous medium (Section 4.2.1.3.1.1). Use of the discrete fracture model approach has been limited to modeling studies that support understanding of thermal-hydrologic processes.

Another category of alternative models involves the manner in which the network of fractures in the host rock is represented by a continuous medium. The thermal-hydrologic models described here represent fracturing using a dual-permeability continuum approach, based on the active fracture concept, which is also used in the unsaturated zone flow model (Section 4.2.1.3.1.1). The dual-permeability approach controls the movement of liquid and gas between fractures and the adjacent intact rock. Other available approaches include dual-porosity models and the equivalent single-continuum model (Hardin 1998, Section 3.3). The need for dual-permeability has been demonstrated by comparison to field thermal test data (Hardin 1998, Section 3.4); other approaches have been determined to provide less realism than the dual-permeability approach.

Alternative models for potential permanent changes in thermal and hydrologic properties of the host rock may be summarized as follows:

- Heating, cooling, and resulting water movement occur in a system with fixed thermal and hydrologic properties (such as porosity, permeability, and thermal conductivity). Properties of the rock may vary with temperature and water saturation but return to pre-repository values after the temperature returns to ambient levels.

- The same processes occur, but thermal effects permanently alter certain properties of the host rock through the action of coupled processes. For example, thermal-hydrologic-chemical coupling may change the hydrologic properties because of dissolution and precipitation of minerals in different regions.

The understanding of thermal-hydrologic-chemical effects on flow is summarized in Section 4.2.2.3.3. The model results indicate that changes in fracture porosity and permeability caused by chemical dissolution and precipitation will be minor compared to total porosity and permeability; hence, the first conceptual model (i.e., stationary properties) is selected as the most credible. This is the conceptual basis for both the mountain-scale thermal-hydrologic model and the multiscale thermal-hydrologic model.

As noted in the previous Section 4.2.2.3.5, supplemental studies have addressed additional alternative models:

- Supplemental studies implemented an alternative seepage method. Instead of using percolation flux as input to the seepage abstraction model, the unsaturated zone seepage model is used, incorporating new models for focusing seepage flow along discontinuities (e.g., faults) and episodic flow (BSC 2001a, Section 4.3.5).

- Supplemental studies implemented effects of mountain-scale gas-phase convective circulation and the movement of water vapor along the axis of emplacement drifts from warmer to cooler regions (BSC 2001a, Sections 5.3.1.4.4 and 5.3.2.4.6).

- Supplemental studies implemented effects of vapor storage and altered heat capacity within lithophysal cavities (porosity) of the Tptpll unit (BSC 2001a, Sections 5.3.1.4.1 and 5.3.1.4.9).

- Sensitivity studies incorporated drift-scale heterogeneity such as the influence of drift-scale heterogeneity of fracture properties, including permeability, porosity, and capillary properties (BSC 2001a, Section 5.3.1.4.2).

Supplemental analyses employing alternative models substantiate the overall model and analytical results of the TSPA-SR model (BSC 2001b, Sections 3.2.2 and 4.2.2).

Drift-Scale Thermal-Hydrologic-Chemical Processes and Models—A model proposed by Matyskiela (1997) suggests that silica precipitation in the rock matrix adjoining fractures will strongly reduce the permeability of the matrix, resulting in significantly decreased imbibition of percolating waters. The time required for strong sealing by silica was estimated for volcanic glasses under saturated conditions. Matyskiela (1997) observed complete filling of pore spaces with silica at fracture–matrix interfaces around a basaltic magma intrusion, the 50-m (160-ft) wide Papoose Lake sill, in the Paiute Ridge area of the Nevada Test Site. He estimated that fracture flow could be enhanced five times in magnitude with the sealing of the matrix pores (Matyskiela 1997, pp. 1117 to 1118). Formation of a silica cap by plugging of fractures with siliceous minerals, as predicted by recent simulations conducted for the potential repository at Yucca Mountain (Hardin 1998, Section 8.5.1), is the opposite behavior. More recent simulation modeling (CRWMS M&O 2000al, Section 3.3.3.5) has shown that fracture plugging will be of limited importance, given estimated fracture porosity of 1 percent.

Lichtner et al. (1999) showed that for a given matrix porosity, fracture plugging depends on the fracture porosity and the particular silica mineral that precipitates. The two-phase numerical simulation results suggest that at distances of tens of meters from the larger Paiute Ridge intrusion in their study, prolonged boiling conditions were established for times on the order of several thousands of years. Amorphous silica, with its higher solubility, is more readily transported by water and therefore produces the largest decrease in porosity, followed by chalcedony and quartz. For substantial sealing of fractures, a very small value of the fracture porosity is necessary. Lichtner et al. (1999) questioned the conclusions of Matyskiela (1997).

Comparison of the geochemical environment around a potential repository at Yucca Mountain with the geochemical environment around a basaltic magma intrusion is provided in supporting documentation (CRWMS M&O 2000c, Section 3.10.9). As discussed in Section 4.2.2.3.3, models of permeability changes due to mineral precipitation indicate that any such changes will be minimal. The sealing effects of silica deposition will probably be less developed at Yucca Mountain because (1) devitrified tuff reacts slowly compared with volcanic glass, (2) unsaturated fractures have less wetted surface area, and (3) the silica concentration in condensate draining through fractures will probably be limited by reaction rate processes.

As noted in Section 4.2.2.3.5, supplemental studies have addressed additional alternative models, including:

- Alternative initial water and gas compositions boundary conditions (BSC 2001a, Section 4.3.6.5)
- Alternative representation of the host rock, including the explicit representation of the Tptpll lithophysal unit mineralogy (BSC 2001a, Section 6.3.1.4.3).

Supplemental analyses employing alternative models substantiate the overall model and analytical results of the TSPA-SR model (BSC 2001b, Section 3.2.4.2).

Drift-Scale Thermal-Hydrologic-Mechanical Processes and Models—Alternative approaches fall into two categories: continuum versus discrete fracture models and method of coupling thermal-mechanical results to hydrologic flow. Both continuum and discrete fracture models have been used on the project. The continuum approach is satisfactory for calculating spatially averaged stress fields but is unable to resolve fracture displacements that affect permeability. The discrete fracture method can calculate movement of a significant number of representative fractures, which can then be related to permeability change.

Fracture displacement through normal or shear movement results in aperture change. The aperture change can be used to calculate both fracture porosity and fracture permeability, based on assumptions about fracture geometry. The approach used in Section 4.2.2.3.4 was to calculate fracture permeability change directly from fracture aperture change, using an empirical relationship based on laboratory studies. An alternative approach, used for thermal-hydrologic-chemical modeling in Section 4.2.2.3.3, assumes a fracture geometry (parallel plates) and calculates permeability change from theoretical considerations.

As noted in Section 4.2.2.3.5, supplemental studies have addressed additional alternative models, including:

- A revised and extended distinct element analysis and a fully coupled thermal-hydrologic-mechanical continuum model (BSC 2001a, Section 4.3.7)
- A simplified cubic block conceptual model and alternative empirical nonlinear relationships to calculate permeability from porosity (BSC 2001a, Section 4.3.7).

Conclusions from the supplemental studies are similar to those reached for the TSPA-SR model: permeability changes are within the range of the ambient seepage model, and thus uncertainty is already captured in the TSPA-SR model (BSC 2001a, Section 4.3.7.5).

4.2.2.3.7 Model Calibration and Validation

Mountain-Scale Thermal-Hydrologic Model—There are no directly applicable data for validation of the mountain-scale response to thermal loading associated with the potential repository. However, numerical models of geothermal and petroleum systems can be validated from a wealth of field-scale testing and geothermal production data. The validity of mountain-scale model predictions is demonstrated by corroborative results from the modeling of analogue systems, from previously published unsaturated zone modeling studies, and from field-scale thermal tests in the Exploratory Studies Facility.

Table 4-15 in Section 4.2.2.2.3.3 lists selected geothermal systems (and, where available, analyses of those systems) that are comparable to the mountain-scale model. Applications for thermal-hydrologic modeling include detailed studies of the genesis, production history, and future performance of geothermal fields. Justification for the modeling approaches used in the mountain-scale thermal-hydrologic model is found in the successful modeling of fluid and heat transport in large natural subsurface systems for which extensive field data are available. The magma intrusion analogues for thermal-hydrologic-chemical processes are discussed in Section 4.2.2.3.5. In addition, models for the recently completed Single Heater Test (Tsang and Birkholzer 1999) and the ongoing Drift Scale Test (CRWMS M&O 2000c, Section 2.2.4) use the same approach and input data as the mountain-scale model. In summary, the mountain-scale thermal-hydrologic model is considered valid because of its similarity to the models developed for field tests and the demonstrated validity of the geothermal analogue models.

Multiscale Thermal-Hydrologic Model—The multiscale thermal-hydrologic model uses a method based on industry-standard finite-difference software that includes both mass and energy balances. Model documentation addresses input data, assumptions, initial and boundary conditions, software, uncertainties, and other information required to replicate the model results.

Several validation approaches are used for the multiscale thermal-hydrologic model, including comparison of thermal-hydrologic modeling with results from the Large Block Test and the Drift Scale Test and comparison of multiscale thermal-hydrologic model results with mountain-scale thermal-hydrologic simulation, as described below. These comparisons are discussed in more detail in supporting documentation (CRWMS M&O 2000cf, Section 6.13).

Thermal-Hydrologic Models of the Large Block Test—A similar modeling approach was used to simulate the entire history of the Large Block Test (CRWMS M&O 2000cf, Section 6.13.1). As an example of model comparison with data, Figure 4-69 shows simulated borehole temperature profiles compared to observed temperatures. Evaluation of goodness-of-fit to measured temperatures shows accuracy of a few degrees Celsius.

Figure 4-70 shows the simulated and measured liquid-phase saturation profiles along another borehole in the Large Block Test. The simulated dryout zone develops more slowly than observed, but the

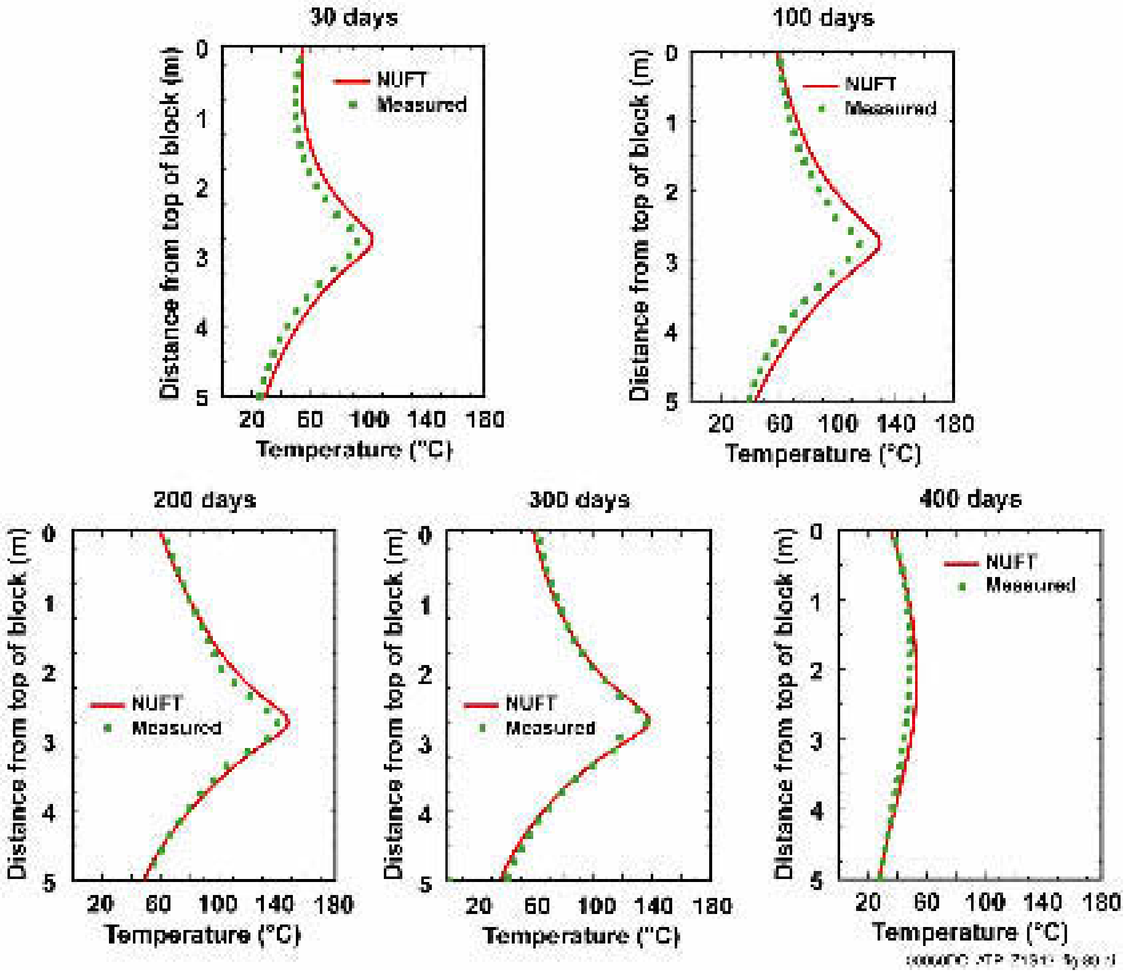

Figure 4-69. Comparison of Simulated and Measured Temperature Profiles along Large Block Test Borehole TT1, at Five Times from 30 to 400 Days

See Figure 4-45 for the location of Borehole TT1. Source: CRWMS M&O 2000cf, Figure 6-65.

difference resolves with time. At later times, the model is in close agreement.

Thermal-Hydrologic Models of the Drift Scale Test—Thermal-hydrologic modeling of the Drift Scale Test heating period, from startup to the present, was compared to observations (CRWMS M&O 2000cf, Section 6.13.2). As an example of model comparison with data, Figure 4-71 compares the simulated and measured temperatures along an observation borehole. The model results are in close agreement with measured temperatures, only slightly overpredicting temperatures in the dryout zone and slightly underpredicting temperatures in the sub-boiling zone.

In general, close agreement with observed temperature in the sub-boiling zone indicates that heat flow there is dominated by conduction and that the value of thermal conductivity is reasonable. Close agreement in the region close to the heated drift indicates that (1) thermal radiation is adequately represented inside the heated drift, (2) heat flow in the boiling and above-boiling zones is dominated by conduction, and (3) the value of thermal conductivity in this region is reasonable.

Comparison of the Multiscale Thermal-Hydrologic Model with the Mountain-Scale Numerical Model—Figure 4-72 compares the drift-wall temperature predicted by the multiscale thermal-hydrologic model with temperatures predicted by east–west cross-sectional mountain-scale thermal-

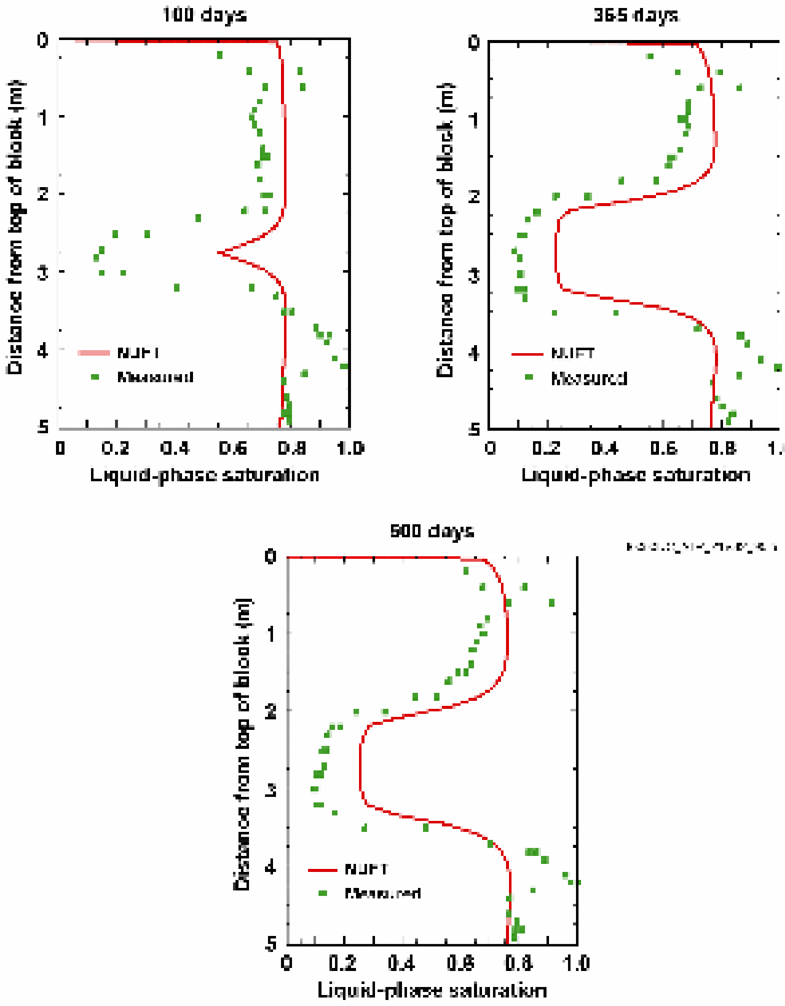

Figure 4-70. Comparison of Simulated and Measured Liquid-Phase Saturation Profiles along Large Block Test Borehole TN3, at Three Times from 100 to 500 Days

See Figure 4-45 for the location of Borehole TN3. Source: CRWMS M&O 2000cf, Figure 6-66.

hydrologic models (for details, see CRWMS M&O 2000cf, Section 6.13.3). The mountain-scale thermal-hydrologic model is coarsely gridded, so the comparison is limited to drift-wall temperature from the multiscale thermal-hydrologic model vs. drift temperature from the mountain-scale thermal-hydrologic model.

Before comparing the two approaches (Figure 4-72), it is important to discuss other differences in the models. Differences between the multiscale model and mountain-scale modeling approaches include:

- The temperature predicted by the mountain-scale model is for a grid block that occupies an entire drift, so it produces a lumped representation of drift temperature, whereas the multiscale model resolves temperature differences within the drift.
- The mountain-scale thermal-hydrologic model uses a line-averaged heat source that axially smooths the differences between hotter and cooler waste package locations.
- The initial areal power density (at emplacement) in the multiscale thermal-hydrologic model is 92.3 kW/acre, compared to 99.4 kW/acre in the mountain-scale thermal-hydrologic model.

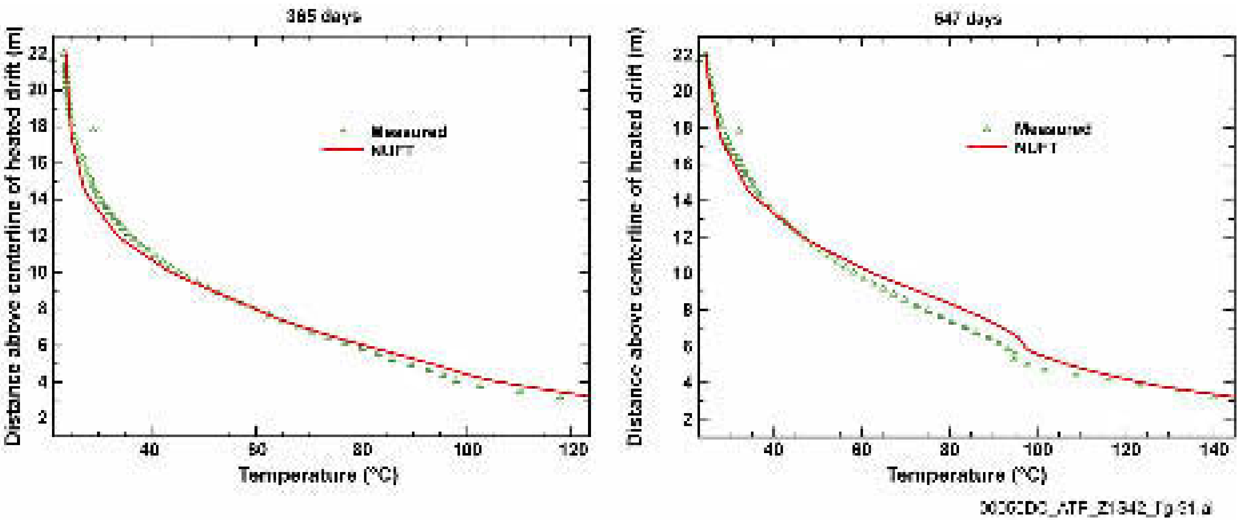

Figure 4-71. Comparison of Simulated and Measured Temperatures along Single Heater Test Borehole ESF-HD-137 at 365 and 547 Days

Source: CRWMS M&O 2000cf, Figure 6-67.

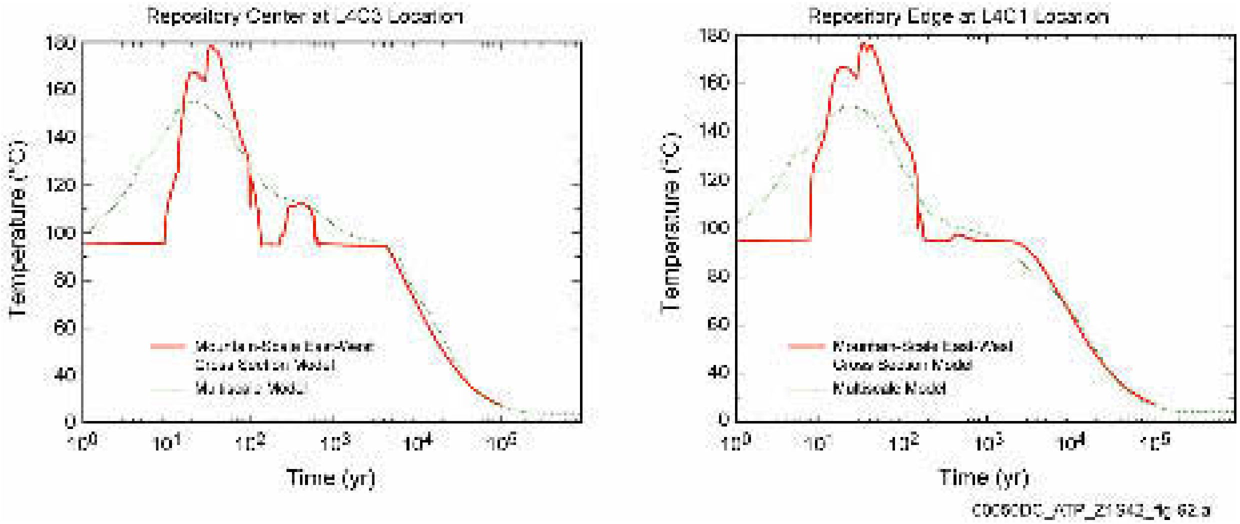

Figure 4-72. Drift-Wall Temperature Predicted by the Multiscale Thermal-Hydrologic Model Compared to the Temperature Predicted by an East–West Cross-Sectional Mountain-Scale Thermal-Hydrologic Model

L4C1 and L4C3 locations are shown in Figure 4-65. Source: CRWMS M&O 2000cf, Figure 6-68.

- The mountain-scale thermal-hydrologic model representation of the heated footprint of the potential repository extends slightly further to the west than in the multiscale thermal-hydrologic model.

Near the center of the potential repository, the approaches predict nearly the same duration of boiling (Figure 4-72, left). Near the edge, the mountain-scale model predicts a longer duration of boiling (Figure 4-72, right). During the post-boiling period, the temperatures predicted by the approaches are in close agreement. During the early heating period, the coarse gridding of the mountain-scale model cannot capture the more rapid changes that the multiscale model predicts. Also because of the coarse gridding, the mountain-scale model tends to overpredict heat pipe behavior. Given the differences in technical approach, the models are in reasonable agreement throughout much of the thermal evolution of the potential repository.

Drift-Scale Thermal-Hydrologic-Chemical Processes and Models—Comparison of model predictions with data from the Drift Scale Test involves (1) modeled patterns of fracture drainage compared to locations where water has been collected during the test, (2) comparison of carbon dioxide concentrations from gas samples, and (3) comparison of the evolution of water composition in boreholes sampled over time.

Simulated distributions of temperature and carbon dioxide concentration are shown in Figure 4-73 for the limited simulation approach (Case 2). The comparison shows that the simulations follow general trends in measured carbon dioxide concentration (CRWMS M&O 2000c, Figure 3.10-5). Two exceptions were when heater power loss occurred temporarily and when the gas samples were acquired at boiling temperatures and condensation occurred during the sampling. Detailed comparison of the modeling results and the measured carbon dioxide concentration data is discussed in *Drift-Scale Coupled Processes (DST and THC Seepage) Models* (BSC 2001o, Section 6.2.7.2).

The simulated pH of water in fractures is shifted to pH 6.5 from an initial pH of approximately 8.3, with the lowest pH values predicted where carbon dioxide concentration is greatest. The predicted shift in pH is similar to that observed in water samples collected from the Drift Scale Test. Chloride concentrations in waters collected from hydrology boreholes are considerably more dilute (a factor of 5 to 10) than the matrix pore water predicted by the modeling. Other species, such as calcite and silica, show similar trends in the modeled fracture water compositions compared to measured water compositions.

In the model simulations, calcite is the major phase forming in the zone above the heaters, although the quantity of calcite is small. Amorphous silica also precipitates but is less abundant than calcite. Direct observation of calcite precipitation or dissolution has yet to be observed in the Drift Scale Test, which is ongoing. However, other indications, such as the composition of water samples, provide indirect evidence for calcite precipitation. Fracture porosity changes predicted for the Drift Scale Test after 20 months are very small (on the order of 0.01 percent of the initial fracture porosity). Such small changes would likely have no measurable effect on the hydrologic properties of the rock.

Drift-Scale Thermal-Hydrologic-Mechanical Processes and Models—Model calibration and validation of fracture displacements due to heating and cooling is done using laboratory and field test results. Calibration includes normalizing models to test results and using observations to determine physical phenomena needed in the models. An example of the latter is the observation of sharp movements in multipoint-borehole-extensometer data at specific times; this observation has resulted in the adoption of a discrete fracture conceptual model in Section 4.2.2.3.4. Validation is the comparison of calculated results to test data, with the calculations being done independent of the test data themselves. Both continuum models and discrete fracture models have been compared to test data from the Large Block Test, the Single Heater Test, and the Drift Scale Test; these tests are described in Section 4.2.2.2.3.2.

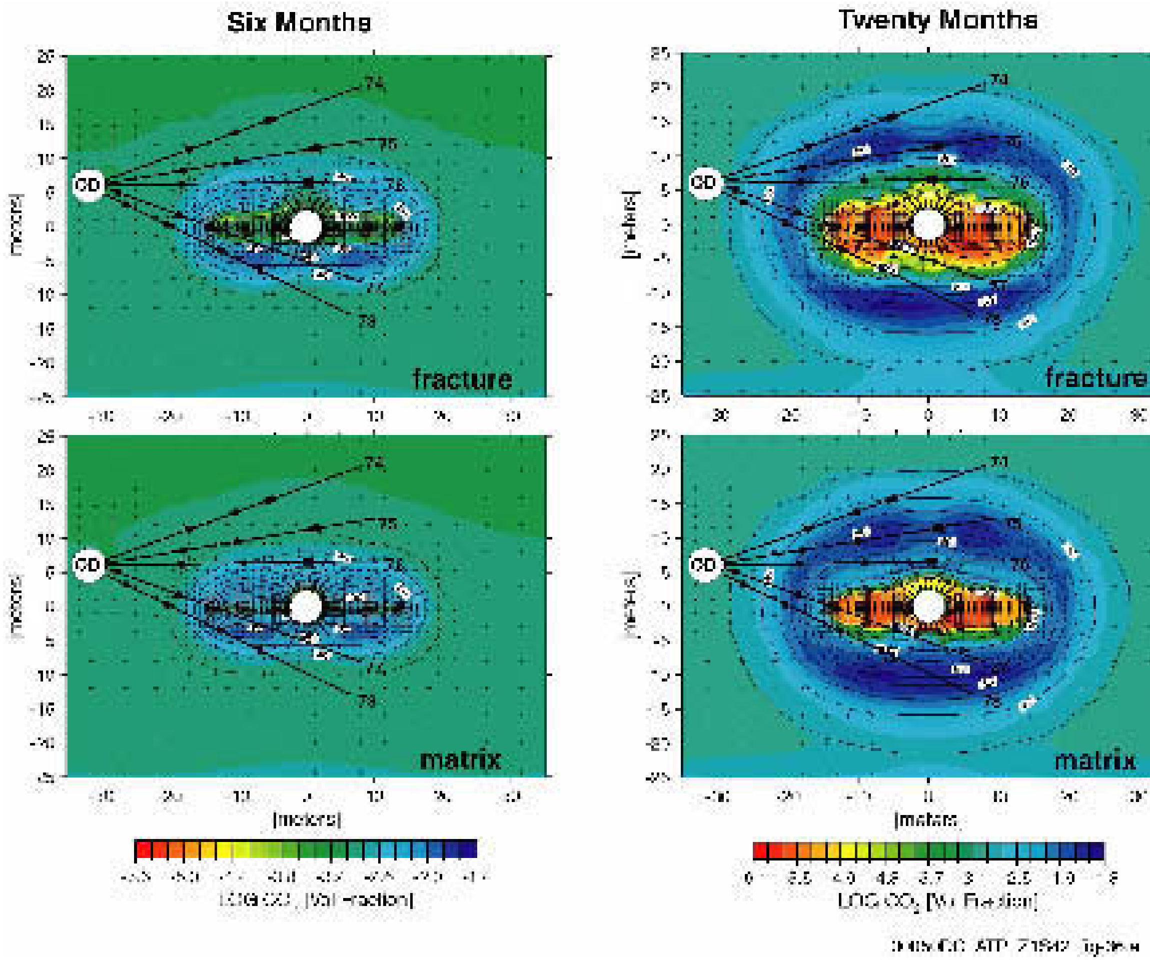

Figure 4-73. Simulated CO_2 Volume Fractions in Fractures and Matrix after 6 Months and 20 Months of Heating During the Drift Scale Test

The white labels indicate locations of isotherms (in °C). These isotherms correspond approximately to the distribution of volume fraction of CO_2, shown by the color contours. The white circle in the center of the plot is the heated drift diameter. "OD" indicates the observation drift from which Boreholes 74 through 78 extend (see Figure 4-52 for the location of these boreholes). Sampling locations in those boreholes are plotted with black dots. Source: Adapted from BSC 2001o, Figures 5 and 6.

4.2.2.4 Total System Performance Assessment Abstraction

Because of the limited thermal effect on water movement at large distances, the mountain-scale thermal-hydrologic model results are not directly included in the TSPA. Abstraction of thermal-hydrologic model results for the TSPA was therefore based on the near-field behavior predicted by the multiscale model.

The mountain-scale thermal-hydrologic model shows that the impacts of repository heating on temperature, saturation, and liquid flux in the unsaturated zone will have limited duration and will be limited to the repository area. Some effects, such as elevated liquid flux associated with heat pipe activity, will be limited to the vicinity of the emplacement drifts. Also, mineralogical alteration of the overlying and underlying hydrogeologic units will be minimal with preclosure ventilation. Accordingly, the thermal-hydrologic effects on far-field flow and transport are not currently considered in the TSPA (CRWMS M&O 2000c, Table 3.13-2).

The purpose of the report *Abstraction of NFE Drift Thermodynamic Environment and Percolation Flux* (CRWMS M&O 2000cc) is to abstract the multiscale, process-level thermal-hydrologic model results (CRWMS M&O 2000cf) so that they can be implemented in the TSPA model. The purpose of the abstraction is to simplify the detailed thermal-hydrologic description of the potential repository that is produced by the multiscale model. An averaging process ("binning") is used to compute these quantities, based on a subdivision of the repository footprint that preserves a wide range of thermal-hydrologic variability. Multiscale model results used directly in support of the TSPA-SR model include waste package temperature, relative humidity at the waste package surface, and the percolation flux in the host rock 5 m (16 ft) above the emplacement drift. Temperature and relative humidity are used for the corrosion model, and percolation flux is used for the seepage model. Time-histories of waste package temperature, percolation flux, evaporation rates, and maximum and minimum waste package surface temperatures are also provided (CRWMS M&O 2000cc, Section 6.3). The abstraction of thermal-hydrologic data represents the potential variability and uncertainty in thermal-hydrologic conditions. It provides a quantitative description of thermal-hydrologic variability (i.e., from variability in the host rock unit, edge proximity, waste package type, infiltration rate, and climate state) and also incorporates uncertainty associated with the infiltration (i.e., lower, mean, and upper).

Abstraction of predicted water and gas compositions for the mean infiltration rate (with climate change), including both limited and full mineral suite simulations, is summarized in Section 4.2.3.4. Also, since the predicted thermal-hydrologic-chemical coupled effects on flow properties are relatively small, the effects on seepage are not included in the TSPA-SR.

The abstracted seepage model used in TSPA-SR performance assessment calculations did not include changes in permeability due to thermal-mechanical effects. This approach was based on *Near-Field Environment Process Model Report* (CRWMS M&O 2000al, Section 5.5) and was confirmed by supplemental TSPA analyses (BSC 2001a, Section 4.3.7.4.4).

4.2.3 Physical and Chemical Environment

The lifetimes of the drip shield and waste package will depend on the environmental conditions to which they are exposed: the in-drift physical and chemical environment (CRWMS M&O 2000a, Section 3.3). Once a waste package is breached, the transport of radionuclides released from the waste form also depends on the environment in the emplacement drifts.

This section describes estimates of how the physical and chemical conditions in the drifts are expected to evolve with time, based on the thermal operating mode described in Section 2. The description is based on the estimated response of the host rock to heating and on data concerning behavior of the engineered materials used to construct the potential repository. The estimates are based primarily on results from laboratory and field-scale testing, supplemented by observations from natural and man-made analogues.

As noted in Section 4.1.4, the DOE is evaluating operation of the repository at lower temperatures. Operating the repository at lower temperatures may change the evolution of the physical and chemical conditions in the drifts described in this section. The data and analytical results presented in this section reflect the effects of higher-temperature operating mode conditions, specifically the process models and abstractions employed in the TSPA-SR model (CRWMS M&O 2000a). Alternative thermal operating modes and supplemental uncertainty evaluations related to the in-drift physical and chemical environment models are described and summarized in *FY01 Supplemental Science and Performance Analyses,* (BSC 2001a, Sections 6.3.3., 6.3.4, 7.3.1, 7.2.4, and 10.3.4; BSC 2001b, Sections 3.2.4.2 and 4.2.4).

Results of the in-drift models used directly in the TSPA-SR model include time-dependent estimates of the infiltration rate, temperature, and relative humidity at the drift wall, as well as the evolution of the chemical conditions at the drift wall over four discrete time periods: (1) preclosure,

(2) boiling, (3) transitional cooldown, and (4) extended cooldown (CRWMS M&O 2000a, Section 3.3.3.4.2).

Physical Environment—The physical environment is described by the evolution, with time, of thermal-hydrologic conditions in the emplacement drifts. Estimation of the temperature, relative humidity, and rate of evaporation at locations throughout the potential repository is described in Section 4.2.2. The results show that every location in the potential repository could evolve from very dry conditions at temperatures greater than boiling to cooler conditions and increasing humidity. Differences between locations are limited mainly to the timing of these changes—for example, the duration of boiling temperatures on the waste package will depend on its location in the repository layout, local infiltration flux, and the heat output of individual waste packages (see Section 4.2.2.3.2). Cooling, and return of moisture to the emplacement drifts, would occur hundreds to a few thousands of years sooner at the edges of the potential repository, compared with the center. Cooling also would occur sooner at locations where there is greater recharge of water from the ground surface.

The potential for liquid water seepage into the emplacement drifts is described in Section 4.2.1. Seepage is combined with temperature, relative humidity, and evaporation rate to represent the physical environment for the engineered barriers in the TSPA-SR. Diversion of seepage by the drip shield and waste package is described in Section 4.2.5. The potential for condensation under the drip shield during the thermal period is also discussed in that section. A model of the flow of liquid water through breaches in the drip shield and waste package is used to assess advective releases of radionuclides in TSPA-SR. Thermal-hydrology, seepage, and water diversion model results that were developed in Sections 4.2.1, 4.2.2, and 4.2.5 are implicit in the following description of the physical and chemical environment and are not discussed further in this section.

The physical environment also includes the potential for rockfall, which could damage the drip shields or waste packages. The effects of rockfall are estimated based on observations from site characterization and use approaches that represent the effects of heating and seismic loading. Estimates of block size and rockfall frequency have been used to design the drip shield, which is designed to withstand rockfall over its design lifetime and thereby protect the waste package. The approach to estimating rockfall events is also described in this section.

Chemical Environment—Important processes affecting the chemical environment include evaporation and condensation of water, the formation of salts, and the effects of gas composition. During the thermal period, relative humidity will likely control the equilibrium solution chemistry and is therefore a principal descriptor of the chemical environment. The approach to analyzing the chemical environment involves several types of predictions:

- Composition of water and gas in the host rock around the drifts that can enter drift openings
- Composition of waters within the drifts that can further evaporate and form precipitates and salts
- The effect of microbial activity on the chemical environment
- The effects of engineered materials such as steel and cement
- The chemical environment at the surfaces of the drip shield and waste package.

These analyses are complementary and together describe the in-drift chemical environment as it is represented for performance assessment. Each is either incorporated explicitly in TSPA-SR or has been considered to have minor consequences to system performance and is excluded from consideration. The approach for each analysis is described in the following sections.

4.2.3.1 Conceptual Basis

This section describes the conceptual models that form the basis for analytical treatment of processes in TSPA. Although the descriptions may contain statements that appear to be definitive, it is important to recognize that there are uncertainties associated with the selection of appropriate conceptual models. Alternative conceptual models are discussed in Section 4.2.2.3.7. Model results based on the selected conceptual models are generally considered to be best estimates, incorporating uncertainty, such that the models are suitable for use in TSPA.

4.2.3.1.1 Conceptual Basis for the Composition of Liquid and Gas Entering the Drifts

Composition of Liquid Seepage—The chemistry of waters in the host rock will act as a boundary condition on the in-drift chemical environment (CRWMS M&O 2000al, Section 3.4.2). During the thermal pulse, water vapor will move away from the heated drifts while liquid water percolates downward and replaces the water that evaporates in a thermal refluxing process (Section 4.2.2). The percolating waters will contain dissolved chemical species, such as sodium, calcium, sulfate, chloride, carbonate, and silica (CRWMS M&O 2000a, Section 3.3.3.4.2). When evaporation occurs, the chemical species will be left behind in the rock as precipitated minerals and salts.

The areal extent of the dryout zone produced by the higher-temperature operating mode would shrink as the heat output from the waste packages decreased with time. This will cause the region of boiling conditions to slowly converge on the drift openings. Liquid water will tend to sweep through formerly boiling regions, redissolve precipitates and salts, and move them closer to the openings. Soluble salts will tend to be concentrated near the openings. Depending on local hydrologic conditions, this process could cause seepage to be concentrated in soluble salts relative to the ambient (preheating) water composition.

With seepage, salts such as calcium carbonate and sodium chloride can form in the drifts (for example, from dripping and evaporation) directly on the drip shield or waste package. In the TSPA-SR model, only a fraction of the waste package locations in the repository would be affected by seepage (Section 4.2.1), especially during the thermal pulse when the conditions are relatively dry (Section 4.2.2). Without seepage, the effects of chemical processes in the host rock on the in-drift chemical environment will be limited to the gas composition. Seepage will be more likely in the future as the climate changes to the cooler, wetter, glacial-transition conditions discussed in Section 4.2.1. However, by the time the effects of this climate change propagate down to the host rock, cooldown will have progressed so that the drip shield temperature will be below boiling throughout the potential repository (CRWMS M&O 2000cf, Section 6.11.4).

After cooldown, and after soluble salts precipitated during the thermal pulse are redissolved and remobilized, the composition of seepage water will become increasingly similar to the ambient percolation in the host rock units. Some minerals precipitated during the thermal pulse may be stable, or slow to dissolve, but effects from such minerals are incorporated into the thermal-hydrologic-chemical model (BSC 2001o, Section 6.1).

Composition of the Gas Phase—The gas-phase composition in the host rock will also act as a boundary condition on the in-drift chemical environment (CRWMS M&O 2000a, Sections 3.3.3.2.3 and 3.3.3.4.2). The gas composition will initially be similar to atmospheric air, but during the thermal pulse, the gas phase will be strongly modified by evaporation of water and by interaction with carbon dioxide in waters and carbonate minerals (BSC 2001o, Section 6.2.7.2). Change in the in-drift gas flux and composition will affect water pH, including water that may occur on the surface of the drip shield or waste package (CRWMS M&O 2000ck, Section 6.2.4; CRWMS M&O 2000a, Section 3.3). Relationships among thermal, hydrologic, and chemical processes in the host rock around the drift openings, and within the drifts, are depicted schematically in Figure 4-74.

Evaporation of water from heating of the host rock will cause much of the dissolved carbon dioxide to be released as gas (the remainder will be precipitated as carbonate minerals). The gaseous carbon dioxide will form a broad halo around the drift openings that encompasses the cooler region where

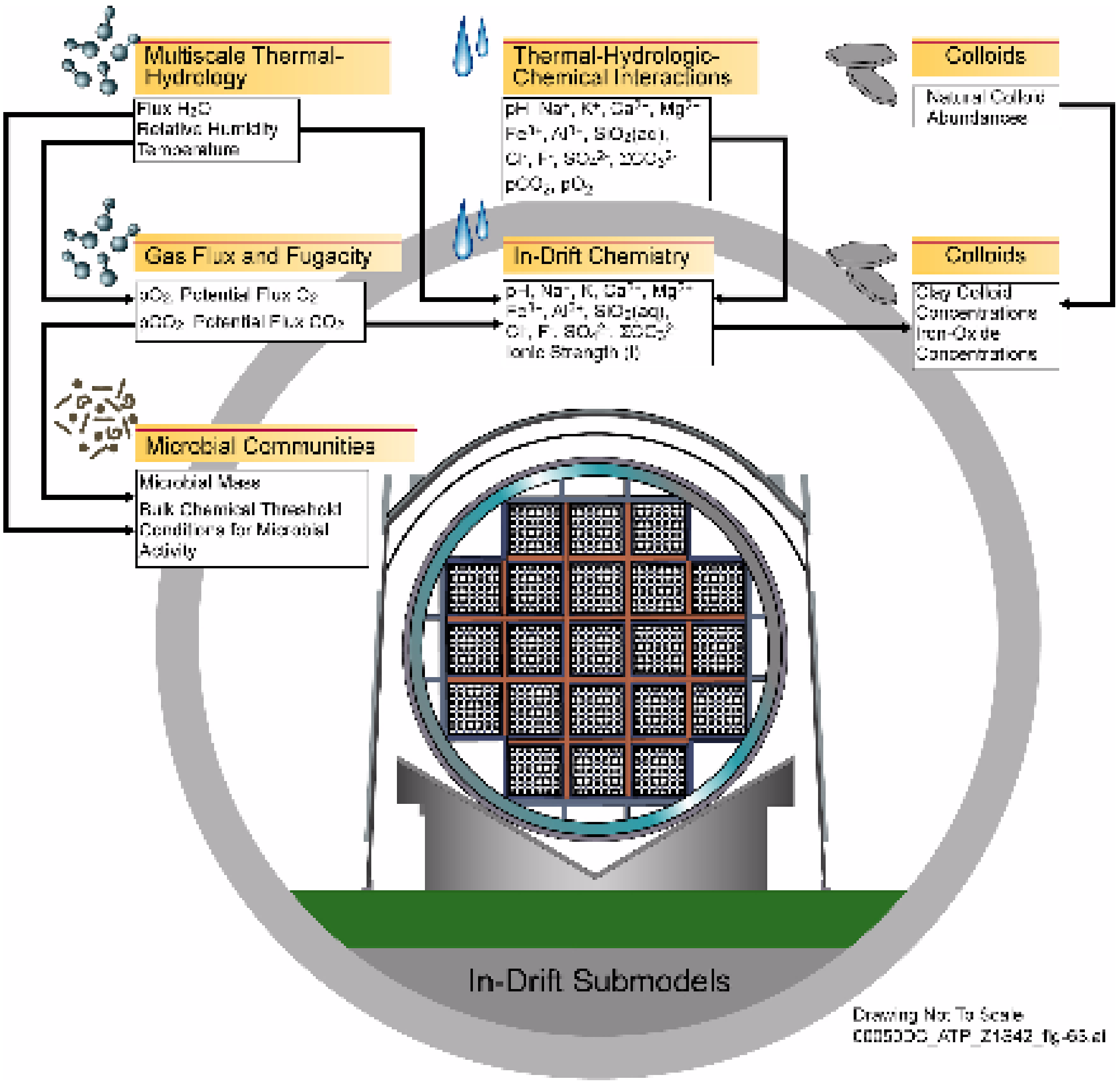

Figure 4-74. Emplacement Drift Cross Section Showing the Processes Considered in the Evolution of the Physical and Chemical Environment, and in the Transport of Radionuclides, within the Emplacement Drifts

Source: Modified from CRWMS M&O 1998g, Chapter 4, Figure 4-1.

water vapor condenses. Condensate will be enriched in carbon dioxide and slightly acidified (CRWMS M&O 2000al, Section 3.6.4.2). In the zone of evaporation closer to the drift openings, calcite and other carbonate minerals will be precipitated but may be redissolved later during cooldown when liquid water returns. Oxygen will exhibit simpler behavior because it is less soluble in water and forms different kinds of minerals. Analyses of uncertainty and the thermal sensitivity of chemical conditions within the drifts are described in *FY01 Supplemental Science and Performance Analyses* (BSC 2001a, Section 6.3).

4.2.3.1.2 Conceptual Basis for Evolution of the Chemical Environment for the Engineered Barriers

At low relative humidity, any minerals or salts that exist in the emplacement drifts will be dry. These minerals and salts may be introduced as ventilation dust, from evaporation of construction water, or from the occurrence of seepage when the drifts are hot and dry. As the relative humidity increases during cooldown, salts will condense to trap water vapor from the air (deliquescence) and form brine. Minerals and salts may occur on a small scale, for example, an evaporated droplet on the surface of the drip shield. Eventually, increasing humidity will cause the brines to capture more water vapor and become diluted. Seepage (where it occurs) will flush soluble salts from the drifts and redissolve the less soluble minerals. After the thermal period, the composition of waters and gases in the emplacement drifts will return to ambient (preheating) conditions (CRWMS M&O 2000as, Section 3.1.2.5.1).

Minerals and Salts Formed by Evaporation—Temperatures well above the boiling point of pure water (96°C [205°F] at the potential repository elevation), and associated low relative humidity, will persist hundreds to thousands of years after emplacement, depending on the location within the repository layout, the local infiltration flux, and the heat output from individual waste packages, as discussed in Section 4.2.2.3.2. These conditions are conducive to evaporation. Seepage into the drifts during this period, if it occurs, may be transient, but the nonvolatile dissolved constituents will accumulate in the drifts as salts and minerals. These solids will include soluble salts with the potential to form brines when relative humidity increases to approximately 50 percent and greater (CRWMS M&O 2000as, Section 3.1.2.5.1). Another source of minerals and salts is dust on the drip shield or waste package surfaces, which could be derived from the rock or from aerosols introduced from the atmosphere by ventilation during the preclosure operational period (CRWMS M&O 2000ck, Section 6.2).

Composition of Waters in the Emplacement Drifts—Temperature and humidity would be slowly varying in the repository, so equilibrium relationships will apply between brine concentration and relative humidity. Thus the relative humidity, which is readily predicted from thermal-hydrologic calculations (Section 4.2.2), is a good estimator of brine composition (CRWMS M&O 2000ck, Section 6.4). As noted previously, all waste package locations will evolve to high relative humidity, but at different rates, so the effect on TSPA is limited mainly to the timing of changes in equilibrium brine composition and seepage.

Where seepage occurs, the rate of seepage entering the drift during cooldown will eventually exceed the rate of evaporation in the drift as the thermal output decays (CRWMS M&O 2000cl, Section 6.2). When this happens, liquid water will begin to flow through the drift. Any brines present will tend to be diluted and flow out of the drifts with the seepage. If seepage is flowing into the drift, then considerable dilution of brines has probably occurred already from the associated humidity. Therefore, the details of seepage mixing with pockets of brine are not critical to predicting the chemical environment.

Microbial Activity in the Emplacement Drifts—Microbial activity is important primarily because of the potential for microbially influenced corrosion of the waste package. Microbes may also increase the rates of degradation for other engineered materials and can contribute to radionuclide transport. Bacteria and fungi, including molds, occur naturally in the host rock and would also be introduced by repository construction and operation. Because of dryness and elevated temperature, heating the rock at the potential repository will arrest microbial activity for time periods on the order of hundreds of years. However, heating will redistribute water so that cooler locations are wetter, which will locally increase the microbial activity. Factors that will limit microbial activity include elevated temperature, low humidity, and availability of nutrients and energy from engineered materials. Engineered materials such as steel may provide metabolic energy sources and limiting nutrients, such as phosphate. Measures to control the use of organic materials during construction and operation will also limit microbial activity (CRWMS M&O 2000as, Section 3.1.2.4).

4.2.3.1.3 Conceptual Basis for the Effects of Engineered Materials on the Chemical Environment

Engineered materials have the potential to affect the chemical environment as they degrade. Drip shield and waste package materials will degrade slowly, and the effects on oxygen availability will be minor. Structural steel in the emplacement drifts will corrode and consume more oxygen, depending on the relative humidity. Cementitious grout will be used to anchor rock bolts in a portion of the potential repository (CRWMS M&O 2000cg) and may contribute cement leachate to the chemical environment.

Degradation of Steel and Alloys—Measured penetration rates for the titanium drip shield and the Alloy 22 waste package outer barrier are small (see Section 4.2.4). These materials obtain corrosion resistance from a passive layer of oxides on the exposed surfaces. The rate of oxygen consumption from maintaining the oxide layer is directly related to the penetration rate.

Steel will be used in roof supports, rails, and beams in the invert that support the drip shields and waste packages (see Section 2.4). These are preclosure structural applications; the steel will readily degrade during the postclosure period when humidity returns. Steel corrosion will begin when the temperature is near boiling and much of the air is displaced by water vapor. The steel is likely to corrode relatively quickly, within a few hundreds to thousands of years. While it is active, steel corrosion may affect the oxygen budget in the emplacement drifts (CRWMS M&O 2000cm, Section 6.2.2).

Cementitious Materials—Cement that will be used in rock bolt installation (like all Portland-based cements) is an assemblage of minerals and other phases, some of which dissolve to produce highly alkaline leachate. The composition of leachate will be determined by the solubilities of cement mineral phases. The phases present in "fresh" cement are more alkaline than those in aged cement because of carbonation and other processes (CRWMS M&O 2000cg, Section 5.3.1). Therefore, the leachate composition can be bounded using readily available information on cement composition. Several factors will act to limit the quantity and quality of leachate produced, including cement carbonation, low grout permeability, limited exposure to seepage flux, and neutralization of leachate by carbon dioxide in the drift environment (CRWMS M&O 2000cg, Sections 6.3.1 and 6.7.5).

Colloidal Particles Produced by Degradation of Engineered Materials—Colloidal particles are important as carriers for radionuclides, particularly isotopes of relatively insoluble elements, such as americium and plutonium. These radionuclides are transported very slowly (or not at all) in groundwater, except for colloidal modes of transport. Colloid generation and radionuclide transport are discussed at length in Sections 4.2.6, 4.2.7, 4.2.8, and 4.2.9. Colloids derived from the host rock will be present in seepage water. Additional colloids will be generated from degradation of engineered materials in the potential repository, including waste forms and other materials within the waste package (CRWMS M&O 2000cn, Section 6.1; CRWMS M&O 2000cg, Section 6.6).

Engineered materials in the emplacement drifts will consist mainly of corrosion-resistant alloys, cement, crushed rock, and steel. Corrosion products of titanium and Alloy 22 are mechanically stable (hence the corrosion resistance of these materials) and are unlikely to form significant colloids. Degradation of cementitious materials can form colloids (Hardin 1998, Chapter 6), but the usage of cement and its exposure to seepage will be limited. The invert ballast material will be crushed tuff derived from the host rock (see Section 2.4.1); the resulting colloids will be similar to colloids introduced with seepage. By contrast, steel in the emplacement drifts will be an abundant source of ferric-oxide colloids that are potentially important for radionuclide transport.

It is anticipated that quantities of colloids will be mobilized as a result of alteration of both the high-level radioactive waste and spent nuclear fuel waste forms. Colloid abundance within a breached waste package will depend on the extent of waste form alteration and the alteration products formed from in-package steel components. Colloid abundance and stability also depend on many environmental factors, including the ionic strength, pH, cation concentrations, colloid content of groundwater entering the waste package from the drift, presence of fulvic and humic acids, and microbe fragments (CRWMS M&O 2000co, Section 1). The colloid source term and transport models are described in Sections 4.2.6 and 4.2.7 of this report, respectively.

Contribution of Engineered Materials to Microbial Activity—As stated previously, microbial activity is important primarily because of the potential for microbially influenced corrosion of the waste package; microbial activity may also increase the rates of degradation for other engineered materials and contribute to radionuclide transport. Microbes exploit chemical reactions (oxidation–reduction) that are rate-limited under abiotic conditions by providing faster alternative reaction pathways that also support cell-building and energy production (CRWMS M&O 2000cp, Section 6.3.1.1). Engineered materials include metals, which are important sources of reactants for these chemical reactions.

Engineered materials in the emplacement drifts will consist mainly of corrosion-resistant alloys, steel, cement, and crushed rock. Each of these can interact with microbes in particular ways, but steel will probably be the most important contributor. Steel will oxidize completely in the first few hundred years after sufficient humidity returns to the in-drift environment; after that, it will contribute little to microbial activity.

4.2.3.1.4 Conceptual Basis for the Environment on the Surfaces of the Drip Shield and Waste Package

Behavior of Water on the Barrier Surfaces—The environments on the surfaces of the drip shield and the waste package will determine the potential for corrosion processes and the penetration rates. Surface chemical conditions will be controlled by temperature, humidity, gas-phase composition (especially oxygen and carbon dioxide), the composition of dripping water, and the minerals and salts that may be deposited.

During the thermal pulse, the drip shield will be warmer than the surrounding in-drift environment in some instances, and the local relative humidity at the surface will be lower than the average humidity in the drift. Under these conditions, any water on the drip shield would tend to evaporate, resulting in concentration of aqueous solutions and precipitation of minerals and salts (CRWMS M&O 2000ck, Section 6.2.3).

The titanium and Alloy 22 surfaces will react with atmospheric oxygen to form thin, resistant layers of metal-oxides (corrosion processes and rates are discussed in Section 4.2.4). These oxide layers will be mechanically stable and chemically unreactive, which confers corrosion resistance to these materials. Because the oxides are chemically inert compared to other species in the environment, they are assumed to not contribute to the chemical evolution of aqueous solutions on the barrier surfaces (CRWMS M&O 2000ck, Section 5).

Waste packages under intact drip shields will be exposed to moisture and chemical species. Humidity will penetrate the air gap between the waste package and drip shield, although the increase of relative humidity at the waste package surface will be delayed because of the warmer temperature there (CRWMS M&O 2000ck, Section 6.2.3). Moisture will form thin films on the surfaces by adsorption or capillary condensation (CRWMS M&O 2000ck, Section 6.3). Minerals and salts will be present in small quantities from dust and aerosols transported in the drift air (CRWMS M&O 2000ck, Section 6.1). If a drip shield is breached, seepage can contact the underlying waste package, which can lead to additional precipitation of minerals or salts on the waste package surface. As the waste package cools, less evaporation will occur on the surface, and accumulation of minerals or salts will be increasingly unlikely.

Potential for Acidic Conditions—There are two mechanisms by which acidic conditions could occur on the surfaces of the drip shield or waste package: radiolysis and localized corrosion. Neither mechanism will be important in the potential repository.

Radiolysis (outside the waste package) will be caused by gamma radiation that penetrates the waste package wall and interacts with air and moisture in the environment to produce small amounts of hydrogen peroxide (CRWMS M&O 2000n, Section 3.1.6.6) and possibly other species, such as nitric acid. Radiolysis inside the waste package is discussed in Section 4.2.4. Several factors will limit the effect of radiolysis on the environment at the waste package and drip shield surfaces. The rate of gamma radiation from spent fuel and other waste forms will decline steeply within the first 1,000 years from the decay of relatively short-lived fission products. Only a small portion of the gamma radiation from the waste package will interact with the air space between the waste package and drip shield; much of this radiation will penetrate the drip shield or be absorbed within it. Acidic compounds formed in the drift environment during the thermal period will likely condense on cooler surfaces such as the drift wall and not on the drip shield or waste package, which will be warmer than their surroundings. If acidic compounds tend to precipitate on surfaces, then the drip shield will afford some protection to the waste package. Finally, the drip shield and waste package materials are resistant to attack by products of radiolysis (Section 4.2.4).

Localized corrosion can, in principle, cause acidic conditions to develop in cracks, crevices, or interfaces where exposure to the bulk chemical environment in the drifts is limited (CRWMS M&O 2000ck, Sections 6.5 and 6.6). Corrosion modes are discussed at length in Section 4.2.4, and localized corrosion is found to be of minor importance for titanium and Alloy 22.

4.2.3.1.5 Conceptual Basis for Rockfall on the Drip Shield

Fractures intersecting emplacement drifts can form "key blocks" that may become dislodged and fall directly onto the drip shields. Key blocks typically form at the crown of the existing excavations, are of minor size, and fall immediately after excavation, prior to ground support installation (CRWMS M&O 2000a, Section 3.3.1). In the design described in Section 2.4.4, the drip shield segments will be pinned together to prevent movement (with allowance for longitudinal thermal expansion and seismic strain). Structural bracing will provide capacity to resist permanent deformation from rockfall. The drip shield segments will have overlapping and interlocking joints to impede water leakage, even with small displacements between segments. The connections between segments will tend to stiffen the structure, so that loads will be shared by adjacent segments. Determination of the size distribution for rock blocks that may fall on the drip shield and analysis of the structural response of the drip shield to rockfall are ongoing activities for which preliminary results are presented in Section 4.2.3.3.5.

4.2.3.2 Summary State of Knowledge

4.2.3.2.1 Composition of Liquid and Gas Entering the Drifts

Ambient Water Composition in the Unsaturated Zone—As discussed in Section 4.2.2.1.3, infiltrating water chemistry could be chosen from either the pore water chemistry in the unsaturated zone at or above the repository horizon or from a more dilute composition found in the perched water or saturated zone. These are referred to as a chloride-sulfate-type water composition and a bicarbonate-type water composition, respectively. As discussed in Section 4.2.2.3.3, the thermal-hydrologic-chemical model assumes the chloride-sulfate-type water as the basis for the initial ambient water composition in fractures in the unsaturated zone.

Composition of Evaporatively Concentrated Waters—Laboratory evaporation tests have been performed using both types of waters to investigate the effects of partial evaporation on solution chemistry and to determine which minerals and salts form as the waters are evaporated completely (CRWMS M&O 2000cg, Section 6.5.2). The bicarbonate-type water has been shown to evolve by evaporative concentration to a brine with high pH, whereas the chloride-sulfate-type water evolves to a brine with a nearly neutral pH. The chloride, sulfate, and nitrate concentrations in these waters tend to increase linearly with evaporation, and precipitate only in the later stages, because they are highly soluble. The major differences in behavior are attributed to the relative abundance of bicarbonate and carbonate among the anions present.

Studies of saline lakes in the western United States show that alkaline sodium-carbonate brines of the type that were produced from bicarbonate-type water in laboratory tests occur in nature (CRWMS M&O 2000cl, Section 6.1.2). Many of these waters occur in volcanic geology similar to Yucca Mountain and have high silica content. These waters also are typically enriched in chloride and sulfate. Similarly, carbonate-poor brines of the type that were produced from matrix pore water in laboratory tests also occur in nature, such as those resulting from evaporation of sea water.

Water samples collected from the rock, in field-scale thermal tests performed at Yucca Mountain, are analogous to waters that would form during the heating of the host rock around the potential repository. The waters were collected where fractures intersected boreholes; therefore, they represent fracture waters that could potentially seep into repository drifts. The composition of such waters has varied with location, temperature, and other conditions but is dominated by condensation and interaction with fracture minerals (CRWMS M&O 2000cg, Section 6.5). The water compositions show that calcite present in the fractures is more readily dissolved than clays, feldspars, quartz, or other forms of silica. The noncalcite constituents of the waters are present in relative amounts that are similar to perched water and water found in well J-13, referred to hereafter as J-13 water (CRWMS M&O 2000cg, Section 6.5). The overall rate of condensation in these tests greatly exceeds the rate of water input from natural percolation, so the waters are dilute. Mixing of condensate with matrix pore waters was limited over the duration of the field tests but may be important over hundreds or thousands of years. From this discussion, it is appropriate to consider a range of water compositions, including bicarbonate-type and chloride-sulfate-type waters, for estimating the effects of evaporatively concentrated water and projecting the evolution of the in-drift chemical environment (CRWMS M&O 2000cg, Section 6.7.4.6).

Ambient Gas Composition—The natural composition of the gas phase in the unsaturated zone at Yucca Mountain is similar to atmospheric air, except that the carbon dioxide concentration is elevated by a factor of three. Elevated carbon dioxide is associated with soil processes near the ground surface and is commonly observed in nature. At other locations where there is more plant activity, the carbon dioxide activity in the subsurface may be an order of magnitude greater than at Yucca Mountain (CRWMS M&O 2000cg, Section 6.2). The oxygen concentration throughout the unsaturated zone is apparently close to atmospheric, indicating there are no natural processes that consume oxygen at rates nearing the rate of potential supply from the ground surface.

Analysis of radiocarbon data from the site, from sampling of pore gas in surface-based boreholes and analysis of core samples, has been used to investigate the natural processes that deliver carbon dioxide to the unsaturated zone (CRWMS M&O 2000cg, Section 6.2). The influx of carbon dioxide dissolved in infiltrating waters, plus that transported in the gas-phase, has been estimated from isotopic mass balance to be in excess of 500 mg carbon dioxide per square meter per year. The results indicate that carbon dioxide is transported in the unsaturated zone by percolating waters and by gas-phase processes, such as barometric pumping.

Effects of Heating on Gas Composition—With heating of the potential repository, carbon dioxide will be released to the gas phase from evaporating matrix pore water (CRWMS M&O 2000al, Sections 3.3.1.2 and 3.3.3). At the same time, the humidity will increase with temperature, and water vapor will displace the air. This will initially cause increased carbon dioxide activity, as observed in field thermal tests, relative to the ambient level for the unsaturated zone. Years later, the carbon dioxide activity will decrease as the temperature approaches 96°C (205°F) (the boiling point at the potential repository elevation) and air is displaced by water vapor. Eventually, during cooldown, the carbon dioxide concentration in the emplacement drifts will approach the ambient level for the unsaturated zone.

Gas-phase convection during the thermal pulse will have an important impact on the fluxes of carbon dioxide and oxygen to the emplacement drifts and on the resulting gas-phase concentrations available for chemical reactions. As the host rock heats up, and the humidity increases, the density of the gas phase will decrease, and buoyant convection may occur. Buoyant convection can occur in porous media, and has been interpreted as the cause for thermal effects associated with hot springs and igneous intrusions (Turcotte and Schubert 1982, pp. 367 to 370). Convection could circulate gas in the unsaturated zone, and thereby move air into the emplacement drifts, decreasing the humidity and increasing the availability of carbon dioxide and oxygen during the thermal pulse (CRWMS M&O 2000cg, Section 6.2.2.2). Increased availability of carbon dioxide will have the effect of buffering evaporatively concentrated, alkaline solutions, particularly above pH 10 (CRWMS M&O 2000cg, Section 6.7.5.3). Increased availability of oxygen will lessen the impact of steel corrosion on the in-drift chemical environment (CRWMS M&O 2000cg, Section 6.3.2.2).

The gas-phase concentration of carbon dioxide in the emplacement drifts during the thermal pulse will also be augmented by liquid water percolation in the host rock. As waters percolate downward toward the potential repository, carbon dioxide will exsolve because its solubility decreases with increasing temperature. If the waters are evaporatively concentrated, more carbon dioxide may be produced. The concentration of carbon dioxide species in such waters can be inferred from the composition of perched waters sampled from field thermal tests (CRWMS M&O 2000cg, Section 6.5) and is predicted using the approach described below.

Approach to Modeling the Composition of Liquid and Gas Entering the Drifts—The modeling approach for seepage and gas-phase composition during the thermal period couples thermal-hydrologic processes with both liquid and gas-phase chemistry. Temperature and evaporative concentration are determined from thermal-hydrology, while dissolution and precipitation reactions are modeled simultaneously (CRWMS M&O 2000c, Section 3.10.5). The thermal-hydrologic-chemical modeling approach is integrated with the unsaturated zone flow model (Section 4.2.1) because the same rock properties and boundary conditions are used. The same coupled model is used in Section 4.2.2 to evaluate the potential for coupled effects on hydrologic properties.

As noted previously, every location in the potential repository will be subject to similar evolution of thermal-hydrologic and chemical processes, but the timing of these processes will depend on local conditions. The principal factors that will control timing are edge versus center locations in the potential repository layout and the local percolation flux (CRWMS M&O 2000cg, Section 6.1). Based on similarity of the process evolution at different locations, it is possible to represent thermal-hydrologic-chemical behavior using a limited set of chemical computational models. The major drawback of such an approach is uncertainty of hundreds to thousands of years in the timing of thermally driven changes in chemical conditions. This uncertainty corresponds to the predicted variability in the duration of elevated temperature on individual waste packages, as discussed in Section 4.2.2.3.2.

For developing and validating this model, results from the Drift Scale Test constrain the thermal-hydrologic response, gas composition, and composition of liquid water in fractures for the first few years of repository evolution. Longer-term evolution is predicted by extrapolation. The concentrations of carbon dioxide and oxygen depend on thermally driven gas-phase circulation, and a range of models and properties are considered and compared (CRWMS M&O 2000cg, Section 6.2).

Water and gas compositions are predicted at the drift wall to represent effects of processes in the host rock and used as boundary conditions for processes in the drift (CRWMS M&O 2000c, Section 3.10.5). These predictions are then used as boundary conditions on a different model for in-drift processes, which uses an approach formulated to accommodate evaporatively concentrated waters with high ionic strength (CRWMS M&O 2000cg, Section 6.7.4.6; CRWMS M&O 2001b, Section 1). Evaluation of the carbon dioxide and oxygen budgets for chemical processes occurring in the drifts and the surrounding host rock shows that chemical reactions will probably not strongly perturb conditions in the surrounding rock (CRWMS M&O 2000cg, Section 6.7). The concentrations of carbon dioxide and oxygen will be uniform within the drift air-space (although relative humidity will vary with temperature) because gas-phase diffusion and convective mixing are rapid compared to the potential rates of consumption of these reactants. Finally, alternative chemical boundary conditions for water composition (i.e., bicarbonate-type and chloride-sulfate-type waters) are used to reflect the present state of knowledge of mobile waters in the host rock (CRWMS M&O 2000cg, Section 6.7.4).

4.2.3.2.2 Evolution of the Chemical Environment

The following discussion describes the summary state of knowledge for processes that will affect the bulk chemical environment in the emplacement drifts. This environment is distinguished from local conditions associated with cracks and crevices, microbial colonies, and within layers of engineered material degradation products.

Minerals and Salts Formed by Evaporation—As Yucca Mountain waters are evaporated to dryness, various minerals and salts are formed in sequence as the solution conditions exceed their solubility constraints. The formation of brines by evaporative concentration of natural waters can be conceptualized as a series of chemical divides, which are caused when salts with limited solubility drop out of solution (CRWMS M&O 2000ck, Section 6.5). The concept of chemical divides is straightforward. When a salt such as calcium sulfate is precipitated from solution during continual evaporation, one or the other of the component species (i.e., calcium or sulfate) will be effectively removed from the water. The remaining one will jointly determine what precipitates next, and so on, in a series of chemical divides. (The situation is more complex for solutions with multiple soluble species, as discussed below.) The complete precipitation of all limited-solubility species is observed in natural waters that have been concentrated by evaporation, such as Owens Lake in southeastern California (CRWMS M&O 2000ck, Section 6.5).

As discussed previously, for particular conditions of temperature and relative humidity, there is a specific extent of evaporative concentration for Yucca Mountain waters, such that the solution is in moisture equilibrium with the gas phase. In other words, the solution will either evaporate or absorb moisture from the air until equilibrium is reached. This equilibrium behavior is well known and has been observed in laboratory tests (CRWMS M&O 2000ck, Section 6.6). Below a critical value of the relative humidity, or deliquescence point, the solution evaporates completely and the resulting salts remain dry. Coligative behavior is observed when solutions are concentrated by boiling; the boiling temperature increases with solution concentration until a limit is reached and the salt precipitates. The deliquescence point and the boiling point have been measured for a number of solutions of pure salts, as shown in Figure 4-75. Various salts exhibit different behavior, but solutions of salts with lower deliquescence points have consistently higher boiling points.

During cooldown of the potential repository, dissolution of salts will occur rapidly when the relative humidity exceeds the critical value for each salt present. Rapid dissolution is consistent with the observation that puddles of dissolved salt (primarily sodium chloride) occur overnight on salt flats when the relative humidity exceeds the deliquescence point for sodium chloride, but the temperature remains above the dew point (CRWMS M&O 2000cl, Section 6.1.4.2). These puddles can then dry up during the day when the relative humidity decreases.

Laboratory evaporation tests have been used to identify the minerals and salts that could form in the emplacement drifts. Tests were conducted using two different water compositions: a bicarbonate-type water and a chloride-sulfate-type water (CRWMS M&O 2000cg, Section 6.5). Evaporation was performed at below-boiling conditions (85°C [185°F]) to represent the behavior of slowly migrating waters in the engineered barrier system. At this temperature, the assemblage of mineral phases resulting from evaporation is controlled by precipitation kinetics. It is thought that the assemblages are representative of potential repository conditions.

The first set of tests using bicarbonate-type water (similar to water from well J-13) showed that the salts formed during complete evaporation included

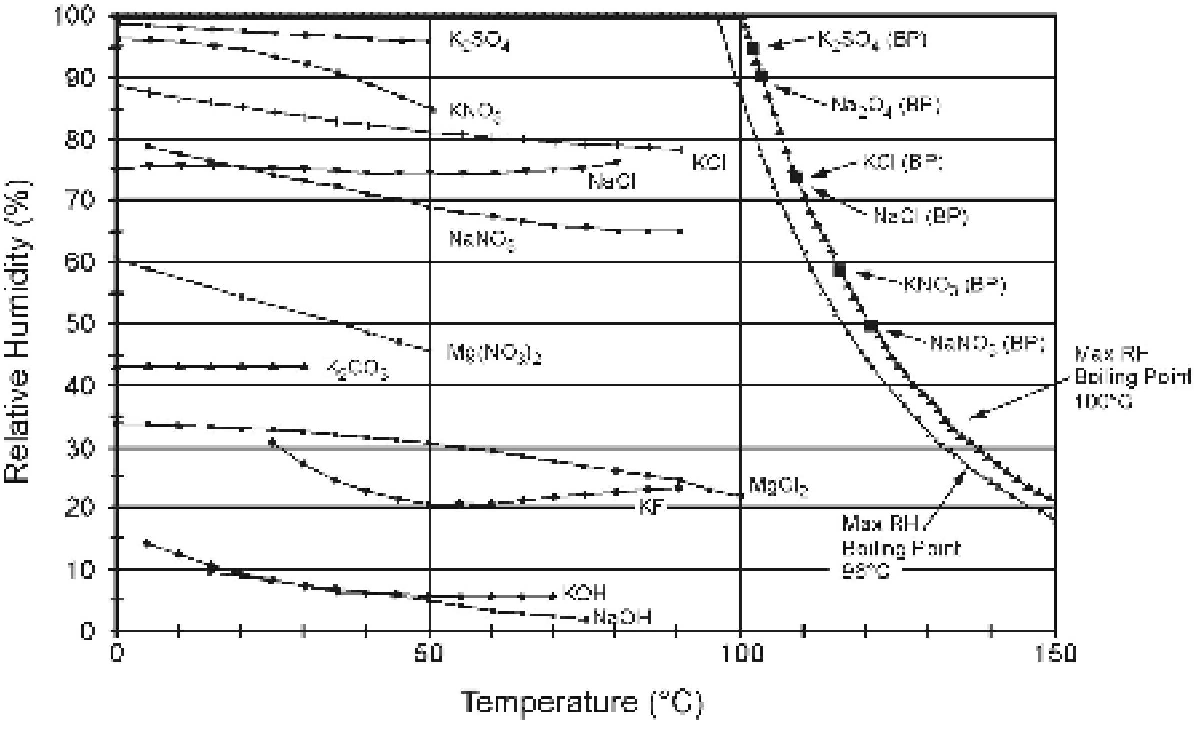

Figure 4-75. Deliquescence Points (Expressed as Relative Humidity) and Boiling Points for Several Pure Salts

This figure plots handbook data for the equilibrium relative humidity, as a function of temperature, for saturated aqueous solutions of some pure salts. Some of these may be present in the emplacement drifts, and these data represent minimum relative humidity conditions when aqueous conditions can occur. Each data curve probably terminates at the boiling curves to the right, but these are gaps in the available handbook data at intermediate temperatures. BP = boiling point; RH = relative humidity. Source: CRWMS M&O 2000ck, Figure 8.

niter, halite, thermonatrite, calcite, and silica (CRWMS M&O 2000cg, Section 6.5). Calcium and magnesium precipitated as carbonates early in the evaporation process, while halite and niter, being more soluble, precipitated when evaporation was nearly complete. The precipitates formed are sensitive to the concentration of carbon dioxide in the environment, which affects the pH environment. The tests provided no evidence of hydroxide precipitates, which would indicate very high pH. When the tests were repeated with tuff particles mixed with the water, similar results were obtained.

Test results for the chloride-sulfate-type water (similar to matrix pore water or sea water) concluded that chloride and sulfate are the major anionic brine constituents, and that carbonate species are substantially less important (CRWMS M&O 2000cg, Section 6.5). As the water was evaporatively concentrated, the pH decreased to approximately 6 or lower. On complete evaporation, chloride and sulfate salts (such as halite and gypsum) predominated. In summary, test results show that calcium and magnesium carbonates, if present, will precipitate early in the evaporation process, while halite and niter are among the last salts to form. Other, additional chloride and sulfate salts will precipitate from chloride-sulfate-type waters.

Composition of Waters in the Emplacement Drifts—Throughout most of the repository performance period, composition of water in the drifts will be similar to that of ambient percolation in the host rock. During the thermal pulse, development of brine compositions that could potentially accelerate corrosion of the drip shield and waste package will depend on the chemical composition in late stages of evaporation.

In the laboratory tests described previously, evaporation of the bicarbonate-type water (similar to J-13 well water) produced a carbonate-rich brine that was highly concentrated in sodium, chloride, sulfate, carbonate, and silica. The pH increased to at least 10 and possibly higher as evaporation progressed. Evaporation of chloride-sulfate-type water (similar to matrix pore water or sea water) produced a carbonate-poor brine that was concentrated in sodium, chloride, sulfate, calcium, and magnesium (CRWMS M&O 2000cg, Section 6.5). Other dissolved components that can be enriched in natural brines include fluoride, bromide, strontium, phosphate, and boron (CRWMS M&O 2000ck, Section 6.1). Laboratory test results have shown that fluoride is not concentrated in brines representing Yucca Mountain waters, probably because these waters contain sufficient calcium and sodium to precipitate fluoride minerals (CRWMS M&O 2000cg, Section 6.5). Other components of natural brines (bromide, strontium, phosphate, and boron) are trace constituents in Yucca Mountain waters and are unlikely to achieve significant concentrations. Thus, the major chemical constituents of concentrated brines in the potential repository drifts will be sodium, calcium, magnesium, chloride, sulfate, and nitrate. For high-pH carbonate-rich brines, silica species and carbonate will also be present.

Brine compositions are outside the range that can be calculated exactly with widely used chemical activity models (i.e., much greater than 1 molal ionic strength). Accordingly, descriptions of brine behavior are more empirical, particularly with multiple dissolved species (not a single salt). The Pitzer approach (CRWMS M&O 2000cl, Section 6.4.2; CRWMS M&O 2000cg, Section 6.7.3) is based on observations of analogous ion interactions and for simulating brine behavior at ionic strengths as high as 10 molal.

Microbial Activity in the Emplacement Drifts—Laboratory testing, combined with microbial test results in the scientific literature, show that threshold conditions for microbial activity and growth are relative humidity above 90 percent, and temperature below 120°C (248°F) (CRWMS M&O 2000cg, Section 6.4.5.1). Field investigations have been performed at Yucca Mountain and at nearby Rainier Mesa to characterize microbial populations in situ (CRWMS M&O 2000cg, Section 6.4). Additional microbial observations from the exploratory tunnels at Yucca Mountain are underway.

Site characterization investigations have shown that in situ microbial growth and activity are limited by availability of water and nutrients, particularly phosphate and organic carbon. In the potential repository environment, microbial activity will also be limited by temperature and radiation (CRWMS M&O 2000cg, Section 6.4). Water will be locally available during the repository thermal evolution, as discussed previously. Phosphate is a trace constituent of J-13 water, probably because the Topopah Spring Tuff contains apatite, a phosphate mineral. Organic carbon may be limiting for some classes of organisms, such as molds, but microorganisms that fix carbon from carbon dioxide are common in rock samples obtained underground at Yucca Mountain; therefore, a source of organic carbon is not required for bacterial growth and activity. Temperature will decrease over time, so microbial activity will be possible within a few hundred years after permanent closure. Radiation from the waste package may sterilize the surrounding environment, but the shielding effect of the host rock will ensure that nearby microbes can recolonize the emplacement drifts. From this discussion, it is evident that microbial activity will occur in the emplacement drifts. The effects of microbial activity on the degradation of the waste package outer barrier material are discussed in Section 4.2.4.3.3. The potential effects on radionuclide transport are discussed in Section 4.2.7.

Approach to Modeling the Evolution of the In-Drift Chemical Environment—In this approach, relative humidity is used as a "master variable" to control the evolution of brines. Initially, the formation of minerals and salts, as seepage waters are evaporated to dryness, is modeled using a normative approach based on the laboratory tests described previously (CRWMS M&O 2000cg, Section 6.5). As relative humidity increases in the emplacement drifts, the salts formed by evaporation gradually become brines and are diluted. For the salts formed from evaporation of bicarbonate-type water (similar to J-13 well water), and considering the behavior of the salts separately and without interaction, deliquescence begins at relative humidity of 50 percent (CRWMS M&O 2000ck, p. 75 and Figure 8). At a greater value of relative humidity, all the salts are considered to be dissolved, and further changes in solution composition are calculated using the Pitzer modeling approach (or other more widely used modeling approaches) as the environment approaches ambient (preheating) conditions. If seepage occurs, it either evaporates completely, forming minerals and salts, or it is partially evaporated and the evaporative concentration effect is accommodated in the chemical modeling approach (CRWMS M&O 2000cg, Section 6.5).

To evaluate the effects of microbial activity on the bulk chemical environment while taking into account the importance of engineered material degradation, an approach is used that incorporates energy balance and mass balance. Threshold conditions determine when microbial growth and activity can resume, then degradation rates for the materials present in the in-drift environment determine the biomass that can be supported. The result of this calculation can be compared with other descriptors of the in-drift environment to assess whether microbial effects are significant (CRWMS M&O 2000cg, Section 6.4).

The same threshold conditions apply to the onset of microbially influenced corrosion of the waste package. While the drip shield and waste package materials are included in the energy- and mass-balance approach, the corrosion rates are developed directly from laboratory tests (see Section 4.2.4).

4.2.3.2.3 Effects of Engineered Materials on the Chemical Environment

Degradation of Steel and Alloys—The product of drip shield corrosion is predominantly titanium dioxide. Alloy 22 corrosion produces oxides of major components nickel, chromium, iron, and molybdenum. These oxides tend to be chemically inert and do not react with other chemical species in the drift environment. They will accumulate slowly, corresponding to general corrosion rates on the order of 10 to 1,000 nm/yr (0.0000004 to 0.00004 in./yr) (see Section 4.2.4). This will consume oxygen at a rate that is negligible compared with the rate of gas flux through the drift openings (CRWMS M&O 2000cg, Section 6.3).

Steel corrosion products are insoluble ferric-oxides or oxyhydroxides. The concentration of ferric iron for aqueous solutions in equilibrium with hematite, goethite, and other iron oxides is very small, comparable to the concentration associated with iron-bearing nontronite clays (CRWMS M&O 2000cg, Section 6.7).

The rate of degradation for structural carbon steel, for vapor-phase conditions representative of the drift environment, has been measured for many samples, at different temperatures, in close proximity to different solutions conditions, such as pH and chloride concentration (CRWMS M&O 2000cg, Section 6.3). The measured penetration rates are on the order of tens to hundreds of microns per year. The corresponding consumption rates for oxygen are comparable to the convective flux of oxygen through the drift openings during the time period when this corrosion will occur.

Corrosion products can increase in volume, and particles can move in the drifts, potentially changing flow characteristics. These effects are neglected because the liquid flux in the drifts will be orders of magnitude smaller than the flow capacity, and redistribution of particulate matter can therefore have only a minor impact on the flow.

Effects of Cementitious Materials—A modified Type-K (Portland-based) expansive cement would be used for rock bolt anchorage in the potential repository. The mix will contain silica fume, plasticizer, and a low water-cement ratio to promote strength, durability, and low permeability (10^{-19} m^2).

The alkaline composition of leachate from rock bolt cement grout will be bounded by equilibrium with portlandite. This approximation is conservative because portlandite will be carbonated over tens or hundreds of years from exposure to carbon dioxide in the gas phase. This behavior is known to occur with long-term exposure of concrete to air (CRWMS M&O 2000cg, Section 6.3).

Colloidal Particles Produced by Degradation of Engineered Materials—The following paragraphs describe laboratory data and field analogue data that are used to estimate the importance of ferric colloids for radionuclide transport.

Naturally percolating, mobile fracture waters have not been intercepted or sampled in the host rock, so groundwater analogues have been used to estimate colloid concentrations in seepage water. Colloids have been sampled by pumping of groundwater from 18 well intervals, from the saturated zone, at or near Yucca Mountain. The concentrations of particles in different size ranges were determined by instrumental analysis (CRWMS M&O 2000cg, Section 6.6). It is assumed that these results are analogous to unsaturated zone fracture waters in the potential repository host rock because the waters are derived from broadly similar rock types and likely have similar compositions. Accordingly, colloids are probably of similar types, consisting mainly of clays and silica.

It is noted that for more concentrated waters with greater ionic strength, such as will be produced by evaporative concentration during the thermal pulse, colloid concentrations are suppressed (Section 4.2.6). As the solution concentration increases, colloid stability decreases (i.e., the maximum possible concentration of colloids, which may vary for different sizes).

Production of colloids from engineered materials will be dominated by steel corrosion products, as discussed previously. The maximum concentration of ferric colloids in seepage waters can be estimated using the groundwater analogue. The affinity of these colloids for radionuclides has been measured in the laboratory (CRWMS M&O 2000cg, Section 6.6). Ferric-oxide colloids were shown to have high affinity for plutonium and americium.

Application to Modeling the Effects of Engineered Materials—The effects of steel on oxygen consumption in the drifts, and radionuclide transport, are modeled using the available information. Consumption of oxygen by steel is modeled by applying the average of measured corrosion rates, subject to a condition that the onset of steel corrosion occurs when the relative humidity is 70 percent. Consumption of oxygen by titanium and Alloy 22 corrosion, and the effects of cementitious materials on the bulk chemical environment, are not included in performance analyses, based on the previous discussion.

Use of groundwater colloids as an analogue for the concentration of ferric-oxide colloids in the drifts is conservative because pumping wells are highly dynamic, and not all colloids in the drift will be ferric-oxide or derived from steel. Also, different types of colloids become unstable in certain pH ranges (point of zero charge), and ferric-oxide colloids are unstable near pH 8, which is very close to the predicted pH of seepage. Use of laboratory test data for radionuclide affinity is also a conservative approach because smaller distribution coefficients would probably be observed in chemical systems with more components, containing anions and cations that could compete with radionuclides for sorption sites.

It is noted that the majority of ferric-oxide corrosion products in the drifts will be immobile in the drift environment and yet exposed to seepage water so that released radionuclides can be immobilized by sorption. The potential for retardation by corrosion products in the drifts was not incorporated into the TSPA-SR model but has been considered in supplemental studies. This supplemental evaluation is described further in Section 4.2.7.

4.2.3.2.4 Environment on the Surfaces of the Drip Shield and Waste Package

Behavior of Water on the Barrier Surfaces—As discussed previously, the deliquescence point defines the minimum relative humidity at which a salt will absorb water from the atmosphere and form a concentrated brine. Figure 4-75 shows deliquescence points for a number of pure salts as functions of temperature. Among the salts which have been identified from evaporation of representative waters, sodium nitrate has the lowest deliquescence point (50 percent). Humidity corrosion of the drip shield and waste package can therefore begin at a relative humidity of 50 percent. This is conservative because deliquescence apparently occurs at greater humidity for mixtures of salts. For example, the deliquescence point for a mixture of salts evaporated from J-13 well water can be inferred from the observed boiling point of a concentrated brine representing the result of evaporating a bicarbonate/carbonate solution. The boiling point for such a brine is approximately 112°C (234°F) (CRWMS M&O 2000ck, Section 6.12.5), which is less than the boiling point of a saturated sodium nitrate solution (Figure 4-75). This means that humidity corrosion of the drip shield or waste package is not actually likely to occur until relative humidity reaches a value greater than 50 percent.

Potential for Acidic Conditions—Inorganic acids could form in small quantities from chemical evolution of brines, or they could be produced in conjunction with localized corrosion processes. These acids, such as hydrochloric acid, have known vapor pressures and will tend to evaporate over time, especially at elevated temperature (CRWMS M&O 2000ck, Section 6.10).

Application to Modeling the Environment on Barrier Surfaces—Consideration of the environment on the drip shield and waste package surfaces is limited mainly to identifying the value of relative humidity at which corrosion will begin. Humidity corrosion begins at 50 percent relative humidity, which is conservative, as discussed previously. The relative humidity is determined from thermal-hydrologic predictions that represent the metallic barriers explicitly.

Once corrosion begins, the water composition is estimated using the approach described previously for the in-drift chemical environment. Possible water compositions range from a concentrated sodium nitrate brine to dilute bicarbonate-type or chloride-sulfate-type waters. The corrosion rates used with these water compositions in the TSPA-SR model are based on laboratory-measured corrosion data for several different water compositions ranging from dilute bicarbonate-type water to concentrated brine, including elevated temperature conditions and both acidified and basified compositions (CRWMS M&O 2000ck, Section 6.12). The selection of these water compositions for corrosion test conditions is central to the approach for representing environmental conditions on the surface of the drip shield and waste package.

Considering the factors limiting production and deposition of inorganic acids and hydrogen peroxide, radiolysis outside the waste package is considered to be of minor importance to corrosion and is not considered in the performance analyses.

4.2.3.2.5 Rockfall on the Drip Shield

The geotechnical parameters required to predict rockfall include data and information collected either by field mapping or by laboratory testing. Joint mapping data for the subunits that constitute the emplacement horizon of the potential repository have been collected from the Exploratory Studies Facility, including the ECRB Cross-Drift (CRWMS M&O 2000e, Section 4.1). Joint strength parameters, including cohesion and friction angle, have been developed from laboratory shear strength test data from core samples and are used to predict both the size and number of fallen rock blocks (CRWMS M&O 2000e, Section 4.1). Rock density data and intact rock elastic properties are used to assess seismic effects and to determine the load applied to the drip shield; these data have also been obtained from laboratory tests performed on core samples (CRWMS M&O 2000e, Section 4.1).

Key block analysis in underground excavations located in jointed rock masses has been considered for a number of design situations. Deterministic methods of block theory in rock engineering were advanced by Warburton (1981) and Goodman and

Shi (1985). The literature provides examples for deterministic analysis of the maximum block size, given the spacing and orientation of three joint sets, and the excavation size and orientation. Subsequent work by other authors has been oriented toward probabilistic risk assessment of key block failure (CRWMS M&O 2000e, Section 6.3). These more recent methods are considered suitable for the analysis of densely jointed and faulted rock masses (i.e., greater than three joint sets) where planar joint surfaces can reasonably be assumed. Such conditions typically exist in the potential host rock units at Yucca Mountain. The probabilistic approach used in the TSPA-SR model is distinguished from traditional key block analysis because it not only assesses the maximum size of key blocks, but it also predicts the number of potential key blocks that will be formed in a certain length of tunnel for any tunnel orientation.

4.2.3.3 Process Model Development and Integration

The discussion of the physical and chemical environment is divided into five parts: (1) the chemical composition of seepage water and gas flux into the emplacement drifts (these are near-field conditions and are bounding conditions to the chemical and physical environment for the engineered barriers); (2) the chemical environment in emplacement drifts; (3) the effects of engineered materials on the chemical environment; (4) the chemical environment on the surfaces of the drip shield and waste package; and (5) the model for the rockfall on the drip shield.

4.2.3.3.1 Modeling the Composition of Liquid and Gas Entering the Drifts

Thermal-Hydrologic-Chemical Seepage Model Approach—This section discusses implementation of the thermal-hydrologic-chemical seepage model. The unsaturated zone flow model and the drift seepage model, which are the bases for thermal-hydrologic modeling, are discussed in Section 4.2.1. This model predicts, at the drift scale, the composition of seepage and the associated gas-phase chemistry for 100,000 years, including the effects of heating.

The effects of heating on gas composition are important for predicting the composition of incoming seepage. The concentration of carbon dioxide in the immediate vicinity of the drift openings will decrease because of displacement and dilution by water vapor. This will be accompanied by decreased carbon dioxide activity in any associated seepage, which will cause pH to increase. In the zone of condensation further from the drift openings, carbon dioxide enrichment will occur, causing pH to decrease. Diffusivity for gaseous species is much greater than for aqueous species, and transport is more rapid. The result is that the region affected by changes in gas composition will be larger than that affected by changes in liquid-phase transport.

Flow of information from various models and data sources to the thermal-hydrologic-chemical seepage model is shown in Figure 4-76. The model uses input from modeling of the Drift Scale Test, the unsaturated zone flow model (CRWMS M&O 2000c), and other sources of geochemical data (CRWMS M&O 2000al, Section 3.3). These inputs ensure consistency between the thermal-hydrologic-chemical seepage model and the other models and data used to calculate drift seepage and the movement of water in response to heating. Other model inputs, including reactive surface areas of minerals, fracture–matrix interaction area, and the mineral volume fractions, are estimated from observed data (CRWMS M&O 2000al, Section 3.2.2).

Comparison with observations from the Drift Scale Test (CRWMS M&O 2000ch) and sensitivity studies on mineral assemblages and water compositions were used to guide development of the model. An example of the comparison of model results and observed data is shown in Figure 4-77. Evolution of the concentration of carbon dioxide in the gas-phase, over time, is compared with model results at four sampling intervals in the Drift Scale Test. For some data, calculated results are shown for nearby points in the model grid. For example, locations labeled “above” or “below” are calculated somewhat above or below the sampled location in the test. Similarly, locations labeled “center” or “end” were calculated near the center or the far end, respectively, of the sampled loca-

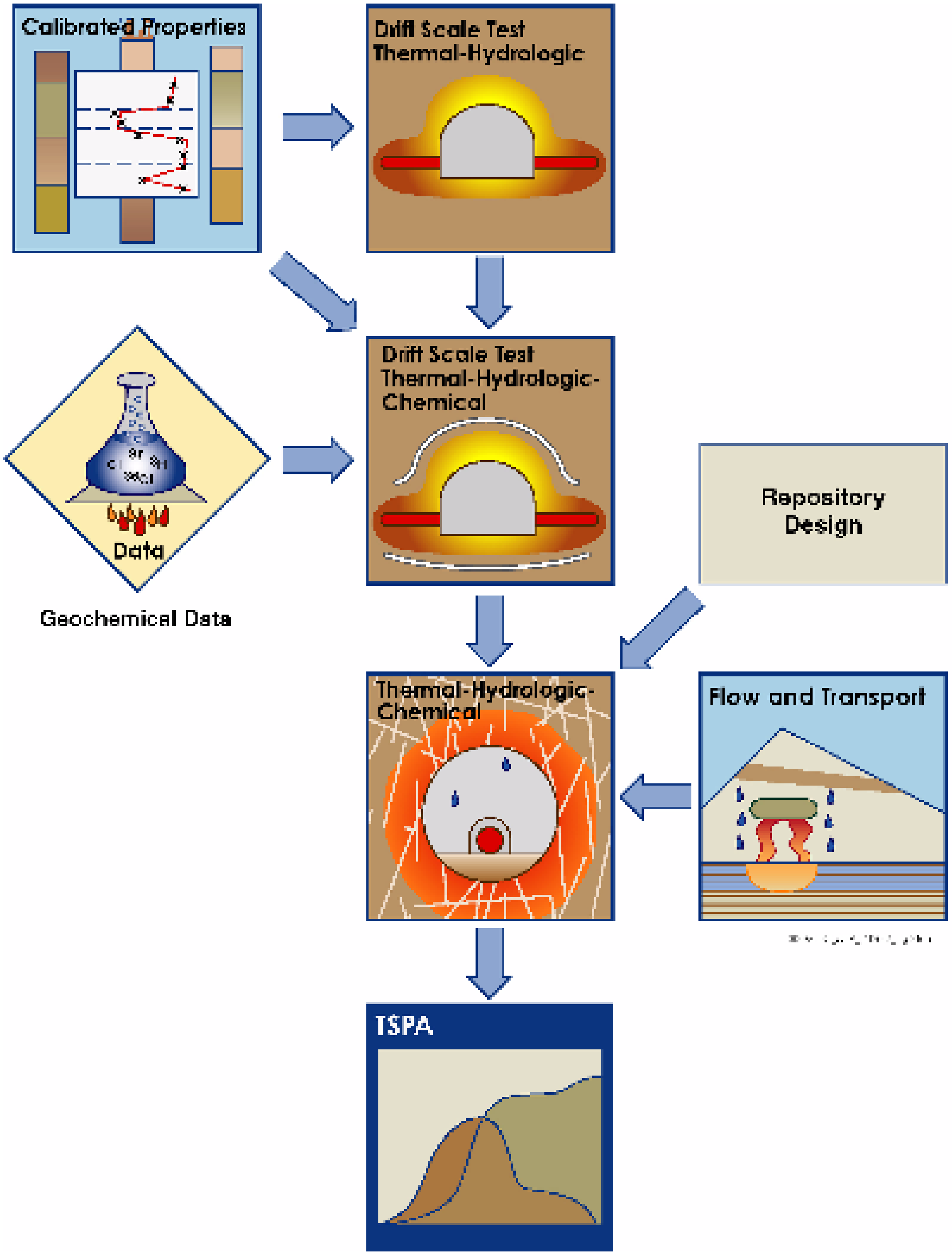

Figure 4-76. Model Diagram Relating Inputs and Outputs for the Thermal-Hydrologic-Chemical Seepage Model, with the Thermal-Hydrologic Drift Scale Test Model, Thermal-Hydrologic-Chemical Drift Scale Test Model, Calibrated Properties Model, Unsaturated Flow and Transport Model, Other Data Input, and Design Information

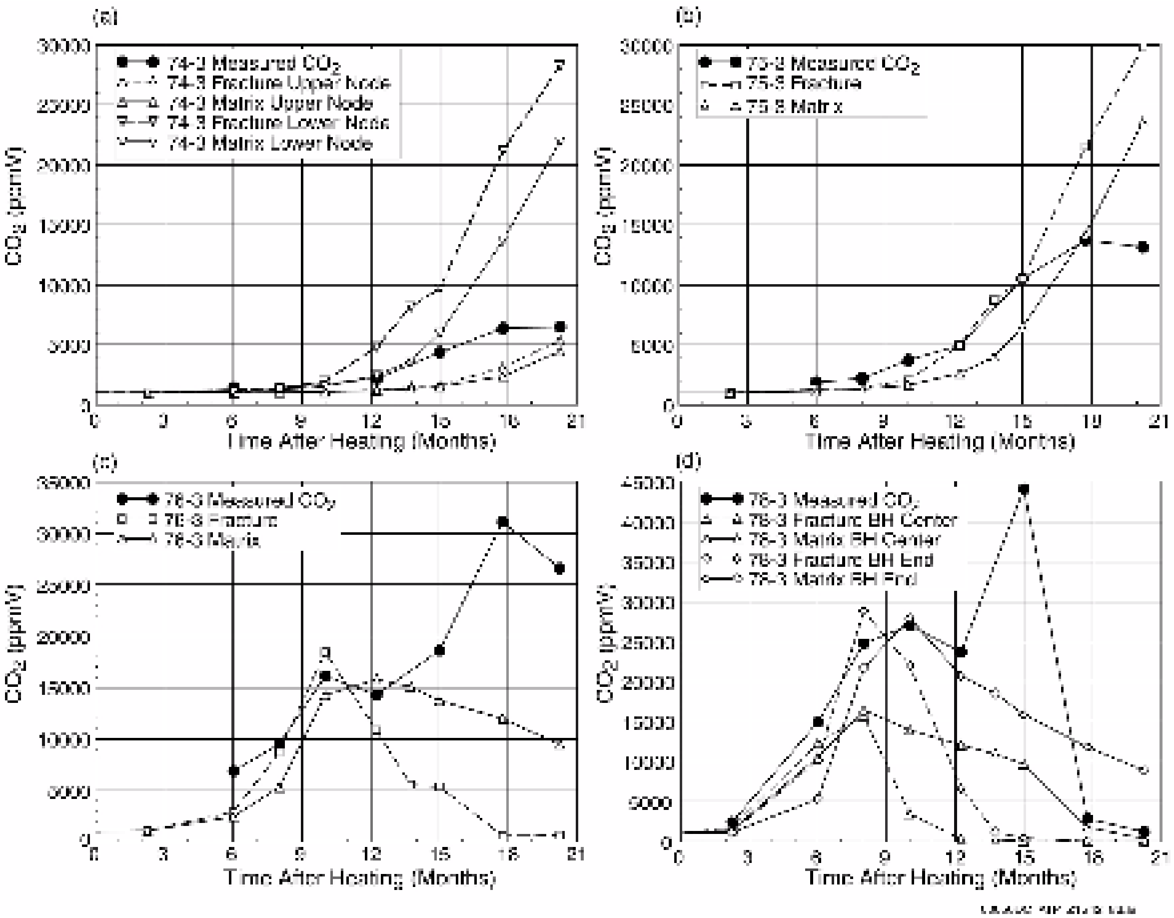

Figure 4-77. Comparison of Modeled Carbon Dioxide Concentrations in Fractures and Matrix to Measured Concentrations in Boreholes for the First 21 Months of the Drift Scale Test

(a) Borehole interval 74-3. (b) Borehole interval 75-3. (c) Borehole interval 76-3. (d) Borehole interval 78-3. Measured data are plotted with black dots; calculated results are shown using other symbols. The model results are from the grid points in the model domain closest to the sampling intervals. The predictive model is based on a limited mineral assemblage that includes calcite, gypsum, and silica phases. See Figure 4-52 for the location of Boreholes 74, 75, 76, and 78. Source: BSC 2001o, Figure 10.

tion. There are comparable trends between the test data and the calculations, and agreement is obtained in an average sense throughout much of the time period modeled.

Thermal-Hydrologic-Chemical Seepage Model Results—The model incorporates elements of the repository thermal operating mode nominally described in Section 2 to represent waste package heating over time, changes in heating from ventilation, heat transfer within the drift, and thermal-hydrologic-chemical processes (CRWMS M&O 2000al). As an example of model results, time profiles for gas-phase carbon dioxide concentrations at three locations around the drift, for one simulation using chloride-sulfate-type water, are shown in Figure 4-78. Carbon dioxide concentrations in fractures decrease significantly during dryout and increase again during rewetting. The increase during rewetting is caused by the dissolution of calcite deposited during dryout and by heating of ambient percolation and condensate waters as they approach the drift opening (the solubility of carbon dioxide in water decreases as temperature increases).

Using the chloride-sulfate-type water as the initial condition, the chloride concentration in fracture

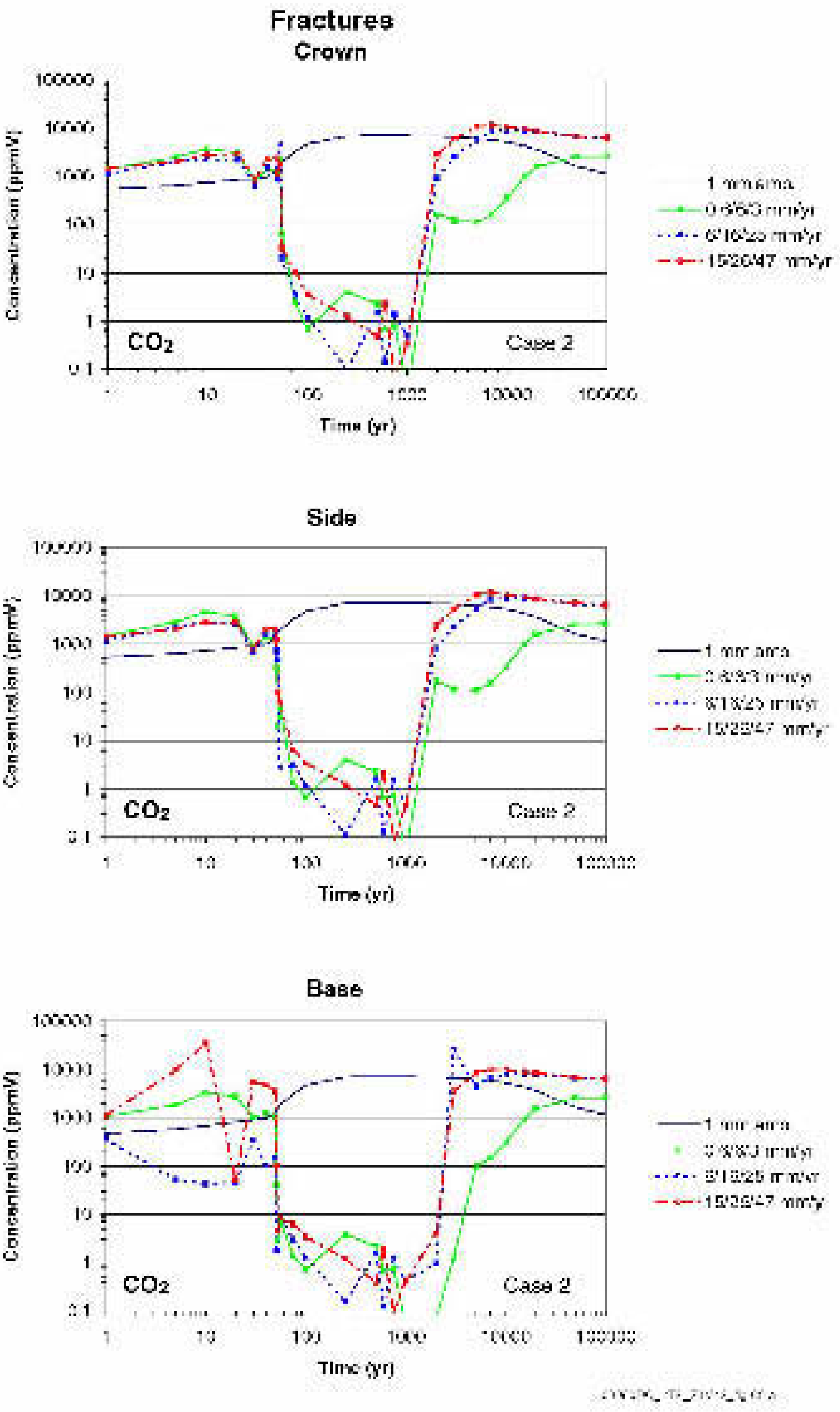

Figure 4-78. Time Profiles of Modeled Carbon Dioxide Concentrations in the Gas Phase in Fractures at Three Drift Wall Locations for Different Climate Change Scenarios

The climate change scenarios are indicated as net infiltration flux values (in mm/yr) for the present-day, monsoonal, and glacial-transition climate states (calcite–silica–gypsum system). For all scenarios, the transitions between these sites occur at 600 and 2,000 years. Source: BSC 2001o, Figure 40.

water immediately above the drifts is estimated to increase approximately fourfold from evaporative concentration. Higher concentrations could occur below the drifts. Upon rewetting, chloride concentrations are estimated to decrease to near-ambient values. The results indicate that seepage water should not be concentrated more than approximately one order of magnitude in chloride, compared to the ambient pore water. For the same simulation, the estimated pH for waters reaching the drift wall ranges from near-neutral (pH 7.2 to 8.3) to sub-alkaline (pH 8.6 to 9.0), depending on the chemical system properties used in the calculation, such as mineral assemblage and gas-phase carbon dioxide (CRWMS M&O 2000al, Section 3.3; CRWMS M&O 2000cl).

4.2.3.3.2 Modeling the Evolution of the In-Drift Chemical Environment

Three complementary modeling approaches are used to describe the formation and behavior of salts under different relative humidity conditions:

- **Normative Precipitates and Salts Model**—Based on empirical data, this model is used to estimate which minerals and salts will form when waters are completely evaporated.
- **Low-Relative-Humidity Salts Model**—The low-relative-humidity salts model describes the behavior of salts when relative humidity is less than 85 percent.
- **High-Relative-Humidity Salts Model**—The high-relative-humidity salts model calculates water composition and dissolution/precipitation reactions for solutions that can occur when relative humidity is greater than 85 percent.

These models are used to determine the timing of in-drift environmental conditions that permit aqueous corrosion and to estimate the composition of waters that can transport released radionuclides.

Normative Precipitates and Salts Model—For waters having compositions similar to either bicarbonate-type water or chloride-sulfate-type water, a set of precipitates is identified that is consistent with the laboratory test data discussed previously. This model describes an assemblage of precipitates formed by complete evaporation. It is approximate in that the laboratory tests may not exactly duplicate evaporation conditions in the potential repository. It is supported by arguments based on thermodynamic data, which indicate that:

- Thermonatrite and calcite are favored over hydroxides such as portlandite because of the presence of sufficient carbon dioxide in the environment.
- Anhydrite is favored to form over gypsum (both forms of calcium sulfate) for the humidity conditions that will be present in the drifts.
- Thenardite (sodium sulfate) and calcite are a more stable assemblage than thermonatrite and anhydrite.

The final species considered in the assemblage is amorphous silica (silicon dioxide), which was detected in all the laboratory samples derived from the bicarbonate-type water. The presence of the tuff would allow for more geochemical processes, such as formation of clays, cation exchange, and silicate buffering associated with tuff dissolution (CRWMS M&O 2000cg, Section 6.5).

Low-Relative-Humidity Salts Model—This model begins at a point in time during the thermal period when the emplacement drifts are dry and at low humidity. Incoming seepage (if it occurs) is completely evaporated, and the salts and minerals that form are determined from the normative approach. As relative humidity continues to increase over time, the salts are allowed to dissolve according to their deliquescent behavior. The amount and composition of brine produced are controlled by the solubilities of the salts and the fraction of each salt that is allowed to dissolve. For the nitrate salts, the entire amount is allowed to dissolve when the relative humidity reaches 50 percent. For the remaining salts, the fraction dissolved is abstracted from the individual salt properties. For simplicity in performance assessment analyses, all of the remaining salts are modeled to dissolve exponentially from zero to unity as relative humidity increases from 50 percent to 85 percent. The timing of relative humidity evolution at different locations in the potential repository is obtained from thermal-hydrologic calculations (Section 4.2.2). At 85 percent relative humidity, all the accumulated soluble salts are considered to be completely dissolved.

High-Relative-Humidity Salts Model—The high-relative-humidity salts model is used for relative humidity greater than 85 percent, conditions for which soluble salts are fully dissolved and the relative rates of evaporation and seepage control the aqueous chemistry. Modeling the behavior of concentrated aqueous solutions (greater than 1 molal ionic strength) is performed using a Pitzer approach, implemented using the EQ3/6 chemical modeling code (CRWMS M&O 2000cl, Section 6.4.2). A modified Pitzer database was developed from existing published data, adding chemical species such as nitrate and silica, and extending the temperature range of applicability to 95°C (203°F). Details are provided in supporting documentation (CRWMS M&O 2000cl, Section 5.3). It is a conservative, approximate model that is used for predicting the composition of water in the emplacement drifts for a time interval during the thermal period when seepage is strongly concentrated by evaporation.

Three sources of experimental data were used for validation of the model (but not for model development or calibration; CRWMS M&O 2000cl, Section 4.1.2). All three studies involved evaporation of synthetic J-13 well water in a beaker open to the atmosphere and maintained at constant elevated temperature. In one study, 30 L (7.9 gal) of synthetic average J-13 water were evaporated to 30 mL and the precipitated solids analyzed. In a second study, the pH of the water was monitored during evaporation, and, in a third, 100-times concentrated average J-13 well water was dripped through a column of heated tuff and final solution composition compared to the initial composition (CRWMS M&O 2000cl, Section 4.1.2).

Results from the high-relative-humidity salts model show that sodium, potassium, chloride, sulfate, and carbonate species simply concentrate without much precipitation. As J-13 water is concentrated to a total ionic content of 10 molal, the pH approaches 10. Species containing silicon, aluminum, calcium, magnesium, iron, and fluoride tend to precipitate in significant amounts relative to their aqueous concentrations. Among the precipitates included in the model, calcite and chalcedony are produced in greatest quantity; magnesium-bearing clay (represented in the model by sepiolite) and fluorite are the next most abundant.

Model for Microbial Activity in the Emplacement Drifts—The approach to assessing the potential effects from microbial activity has two parts: (1) a threshold model for environmental conditions that permit microbial growth and activity and (2) a quantitative model to bound the quantity of biomass, including microbes, that could develop in the emplacement drifts.

Relative humidity, temperature, and radiation dose conditions are combined to formulate threshold environmental conditions for microbial activity. Published results based on extreme behaviors of known organisms are used as a guide where site-specific data are sparse. More precise estimates based on characterization of organisms at Yucca Mountain are unwarranted because of the uncertainty about which types of organisms will be present and the potential for biological adaptation.

Microbial growth and activity does not occur until the local temperature decreases to less than 120°C (248°F) and relative humidity increases to 90 percent. Microbially influenced corrosion of the waste package is conservatively assumed to begin when the relative humidity reaches 90 percent.

The microbial communities model quantifies the abundance and metabolic activity of microorganisms in the engineered barrier system environment. It is based on models used in the Swiss and Canadian nuclear waste programs (CRWMS M&O 2000cp, Section 6). An idealized elemental composition for microbial biomass is used, consisting of carbon, nitrogen, sulfur, and phosphorous in fixed proportions, plus water. The rates of supply for these constituents are input as constant release rates for each natural and engineered material present in the drifts. The other major constraint is the chemical energy available for microbes to grow, which is maximized from possible oxidation/reduction reactions.

The presence of water, nutrients, and energy sources is required for microbial growth and activity. There are three main categories of introduced materials that could furnish nutrients and energy: steels/alloys, cementitious materials, and organic substances (CRWMS M&O 2000as, Section 3.1.2.4.2.1).

Three basic approaches to modeling microbial nutrient and energy balances are possible, based on nutrient balance, thermodynamic energy balance, and chemical kinetics. The microbial communities model (CRWMS M&O 2000cp, Section 6) combines the nutrient and thermodynamic approaches. The available materials are decomposed into their basic elements and combined with the constituents available from groundwater and gas fluxes through the repository. Release of chemical constituents is controlled by estimating the degradation lifetime of each material. The model assumes that all available nutrients and redox energy sources are used for microbial processes and is therefore bounding.

Application of the microbial communities model to the potential repository design shows that approximately 10 grams of biomass would be produced per lineal meter of emplacement drift per year, during the first 10,000 years. Based on this small generation rate, effects on the bulk chemical environment are considered negligible for the TSPA-SR analyses (CRWMS M&O 2000as, Section 5.3.2.4). Localized effects of microbial activity could nevertheless alter the longevity of materials and the transport of radionuclides. For that reason, microbially influenced corrosion of the waste packages was included in TSPA-SR calculations (CRWMS M&O 2000a, Section 3.4.1.6).

4.2.3.3.3 Modeling the Effects of Engineered Materials on the Chemical Environment

Modeling the Effects from Corrosion of Steel and Alloys—Steels and alloys introduced to the potential repository as ground support and other structural materials will degrade with time. The important effects of metal corrosion on the bulk chemical environment, and the approaches used to represent those effects, are summarized as follows.

Oxygen in the drift environment will be consumed, decreasing the partial pressure of oxygen while corrosion is active. This effect is modeled by converting rates of metal corrosion to rates of oxygen consumption and comparing the results with estimates of the available oxygen flux (CRWMS M&O 2000as, Section 3.1.2.3.4).

A corrosion-rate model for structural steel was used to develop estimates of oxygen availability. The potential consumption of oxygen from corrosion of other alloys is also discussed briefly. Corrosion rates for A516 carbon steel have been measured for representative vapor-phase conditions (not immersion), elevated temperature, and proximity to synthetic groundwater with a composition similar to evaporatively concentrated J-13 water. These data are used to represent corrosion of structural steel in the drifts, as there is a paucity of equivalent data for other steels. The rate can vary with temperature, pH, and water composition. In addition, laboratory data for a similar carbon steel composition (CRWMS M&O 2000cg, Section 6.4) suggest an approximate sixfold increase in the corrosion rate once moisture returns to the drifts because of microbial activity. Steel corrosion will be insignificant until the relative humidity exceeds 70 percent (CRWMS M&O 2000cg, Section 6.3.2.2).

Applying measured corrosion rates for structural steel and using environmental conditions representing the potential repository environment yields the following results (CRWMS M&O 2000cg, Section 6.3):

- Steel present in the drifts will completely corrode within a few hundred years, starting at times from approximately 300 to 2,000 years after waste emplacement. (Timing will depend on the duration of preclosure operations and location in the repository layout; steel corrosion can begin at 300 years after emplacement if the preclosure period is

50 years, and corrosion first occurs near the repository edge, which cools fastest.)

- The calculated rate of steady-state oxygen consumption will be replenished by the flux of oxygen that is transported to the drifts by buoyant gas-phase convection.

Results indicate that oxygen partial pressure in the drifts would be decreased but that the flux of oxygen would probably be sufficient to maintain oxic (i.e., corrosive) conditions. In the potential repository, the corrosion rate for structural steel will tend to decrease as the oxygen partial pressure decreases, prolonging the degradation process but moderating the impact on oxygen partial pressure. This model is therefore conservative because the laboratory corrosion data on which the rate model is based were acquired for oxic conditions (CRWMS M&O 2000as, Section 3.1.2.3.4).

The drip shield, waste package, and waste package supports in the design described in this report would be made from titanium, Alloy 22, and stainless steel. Corrosion of these materials will be much slower than for carbon steel and therefore slower to consume oxygen. Consumption of oxygen by corrosion of Grade 7 titanium or Alloy 22 could contribute slightly to depletion of oxygen in the engineered barrier system. However, the potential rate of consumption is a small fraction of the oxygen availability (CRWMS M&O 2000cg, Section 6.3).

Modeling the Effects from Cementitious Materials—The model for the effects of cement grout used in rock bolts is based on dissolution of cement mineral phases and subsequent interaction of cement leachate with carbon dioxide in the drift environment. The results indicate that the potential contribution of cement leachate to the bulk chemical environment will be minor (CRWMS M&O 2000cg, Sections 6.3 and 6.7).

Chemical equilibrium calculations for cement are performed using a mineral assemblage that includes constituents of young cement as a bound on the potential to produce alkaline leachate (CRWMS M&O 2000cg, Section 6.3). Mineral assemblages representing alteration of Portland cement by aging and carbonation are available but tend to produce less alkaline leachate.

The initial composition of water that interacts with cement is assumed to be that of J-13 water, but the potential contribution of influent water chemistry to the leachate is minor because leachate composition (before reaction with carbon dioxide) will be dominated by the cement. Reaction of groundwater with the grout is assumed to be closed (i.e., it does not include reactions with gas-phase carbon dioxide), which maximizes the leachate pH. Biotic processes are also assumed to have a negligible effect on leachate composition because the organic content of the plasticizer admixture probably has very low biological reaction rates (CRWMS M&O 2000cg, Section 6.3).

Once the leachate flows into the drift opening or the surrounding rock, it will be exposed to carbon dioxide in the emplacement drifts, which will moderate the pH. Because of the small amount of leachate compared to the total percolation through the host rock, open-system conditions are used for evaluating this interaction. In addition, contact with silica, such as the cristobalite present in the host rock, will also moderate leachate pH.

The grout permeability is small, which limits chemical interaction with the drift environment while increasing the longevity of the grout to dissolution. Very small flow rates (a few milliliters per year per rock bolt) are obtained using the saturated hydraulic conductivity of the grout. A more conservative bounding approach is used to account for the possibility of grout cracks, allowing higher water contact rates. This approach is based on the ratio of the rock bolt grout cross-sectional area to the drift diameter. This method produces flow rates on the order of a few percent of the total seepage inflow to the drifts.

Results from this model show that prior to contact with carbon dioxide or siliceous minerals, the leachate will be highly alkaline, with a pH value of 11 or greater. This is caused primarily by dissolution of portlandite, which has retrograde solubility (higher solubility at lower temperatures). Buffering on contact with carbon dioxide and near-field rock in the drift environment will result in substantial decrease in leachate pH. Accordingly, elevated pH values from the leachate are unlikely to be present at the drip shield or waste package.

The model does not consider the possibility that grout could break up into fragments, some of which may fall and come to rest on the drip shield. A transient pulse of alkaline leachate could result from such failure, and the current model does not explicitly address rapid leaching. However, the analysis shows that if such leaching occurs during the thermal pulse, the chemical composition of the leachate will be similar to evaporatively concentrated waters that will form in the drift. During and after cooldown, the concentration of carbon dioxide will increase in the drift environment, and cement fragments will be exposed to increased carbon dioxide levels. The potential for strongly alkaline conditions will then be moderated by reaction of leachate with the drift environment. Also, carbon dioxide gas will diffuse into the grout and react directly with the cement. This process is not considered in the current model but will be more important for fragmented grout. Finally, the current model indicates that the quantities of leachate produced are likely to be small, whether or not the grout is fragmented.

Modeling the Effects of Colloids Produced from Engineered Materials—Ferric-oxide colloids with strong affinity for plutonium and americium will be produced from corrosion of steel in the emplacement drifts. The size and concentration distributions of natural colloids observed in local groundwaters are used to represent the behavior of ferric-oxide colloids. This is justified because these waters are similar in composition to seepage waters that are likely in the potential repository (CRWMS M&O 2000al, Section 3.3.2.4). It is conservative because the effect of ionic strength in evaporatively concentrated waters, and the behavior of ferric-oxide at near-neutral pH, will decrease the stability of ferric-oxide colloids. Colloids are discussed further in Section 4.2.7 in the context of the radionuclide transport model.

4.2.3.3.4 Modeling the Environment on the Surfaces of the Drip Shield and Waste Package

Conditions for Aqueous Corrosion and Humidity Corrosion—At permanent closure, the surfaces of the drip shield and waste package will be dry, with relative humidity less than 50 percent, and no humidity corrosion or aqueous corrosion processes active. This condition will continue through the period of peak temperatures. During cooldown, the relative humidity on the barrier surfaces will gradually increase (CRWMS M&O 2000n, Section 3.1.3).

Figure 4-75 shows that aqueous salt solutions on the drip shield and waste package can exist for relative humidity less than 100 percent but greater than the deliquescence point. Analysis of salts formed from laboratory evaporation tests shows that the salt with the lowest deliquescence point is sodium nitrate (CRWMS M&O 2000n, Section 3.1.3.1).

For modeling purposes, it is assumed that sodium nitrate—the salt with the lowest deliquescence point among all the salts likely to be present—will determine the minimum relative humidity at which aqueous conditions can occur (50 percent). Another value of relative humidity is selected to represent the condition at which all salts, including chlorides, sulfates, and carbonates, are dissolved as brine (85 percent). This value is greater than the deliquescence points for all salts that are likely to be present. The low-relative-humidity salts model is used to predict the composition of brines present on the drip shield and waste package surfaces as the relative humidity increases from 50 to 85 percent. This is a conservative approach because waste packages under intact drip shields will be affected only by dust and aerosols, which may be more benign than the brine conditions considered in the model.

The high-relative-humidity salts model is used to calculate the composition of brines as they undergo further dilution at relative humidity greater than 85 percent. If seepage occurs during the thermal pulse, the waters that contact the drip shield and waste package surfaces will be evaporatively concentrated because the relative humidity on the surfaces will be less than in the surroundings. The high-relative-humidity salts model is used to calculate the composition of evaporatively concentrated seepage waters. The degree of evaporative concentration will decrease with time as the relative humidity increases.

The high-relative-humidity submodel of the in-drift precipitates and salts analysis was implemented for relative humidity greater than 85 percent. In this regime, the steady-state water composition is controlled by the ratio of the evaporation rate to the seepage rate; this ratio is always less than one. The submodel calculates water composition, pH, chloride molality, and ionic strength in the repository for several temperatures, relative humidities, relative evaporation rates, and carbon dioxide gas fugacity values (CRWMS M&O 2000cl, Section 6.4.2).

Composition of Aqueous Solutions Used for Corrosion Testing—The exact chemistry of the water that contacts the drip shield and waste package surfaces cannot be known precisely. However, several test solutions have been developed for laboratory corrosion testing of titanium, Alloy 22, and other materials. These solutions were selected to represent a range of dilute and concentrated conditions, pH, and temperatures that could result from evaporative concentration in the repository. The test solutions are described in Section 4.2.4.2.

The chemistry of the waters that contact drip shield and waste package surfaces would vary in a repository, and the test solutions described previously represent a range of possible conditions. Results from corrosion testing with these solutions are discussed in Section 4.2.4.

4.2.3.3.5 Model for Rockfall onto the Drip Shield

The effect of rockfall on the emplaced drip shield was screened from the TSPA-SR model based on the following analysis. *Drift Degradation Analysis* summarizes the analysis of key blocks, including block failure due to seismic and thermal effects (CRWMS M&O 2000e, Section 6), using the probabilistic Discrete Region Key Block Analysis method (CRWMS M&O 2000a, Section 3.3.1; CRWMS M&O 2000e, Attachments VIII through XI).

Based on mapping data and results from key block analysis, the orientation of the emplacement drifts, as discussed in Section 2.1.2, was selected to maximize drift stability (CRWMS M&O 2000e, Sections 1.4 and 6.4). Considering static plus seismic loads, rockfalls were estimated using the probabilistic key-block analysis. The results include probability distributions for the size of fallen key blocks and the number of such blocks per length of emplacement drifts.

Heating and subsequent cooling of the repository host rock would impose stresses, deposit minerals, and shift rock joints. This was represented in the analysis as reduction in joint cohesion from the time of closure until about 2,000 years after closure and thereafter. The resulting changes in estimated rockfall are provided in supporting documentation (CRWMS M&O 2000e, Section 6). Results for combined thermal and static loads are similar to those for combined seismic and static loads.

Given the distribution of key block size, a structural calculation was performed to determine the stresses in the titanium drip shield (BSC 2001l). The analysis considered a range of rock sizes falling onto a 3-m (10-ft) length of drip shield. This length is half that of a drip shield segment and was chosen to take advantage of symmetry and thereby reduce computational effort. A range of rock sizes up to 10 metric tons (approximately 4.15 m^3 [147 ft^3]) is the design basis for the drip shield. For rock sizes up to 4 metric tons, the entire volume of a rock can be located above a 3-m (10-ft) partial-length drip shield. An analysis of the joint geometry suggests that an increase in rock size must occur by an increase in length of the rock block along the drift, rather than an increase in block height (CRWMS M&O 2000e, Attachment IX). The probabilistic key-block analysis showed that the maximum block size could be greater than 10 metric tons, but such large blocks would be relatively unlikely. Probabilistic key-block analysis was performed for the middle nonlithophysal, lower lithophysal, and lower nonlithophysal host rock units. For these units, the proportion of rock blocks simulated that exceeded 10 metric tons ranged from 0 to 5.8 percent (CRWMS M&O 2000e, Figures 27 to 29 and Attachment II). Also, because of their large dimensions, each block would be distributed over more than one 6-m (20-ft) drip shield segment, so the loads would be shared. Using the concept of effective rock mass over a 3-m (10-ft) partial-length drip shield, the maximum rock mass is determined to be 10 metric tons per 3-m (10-ft) partial-length drip shield. In other words, any rock mass greater than 10 metric tons will load a 3-m (10-ft) partial-length drip shield the same as a 10-metric-ton rock. Calculations for the effective rock mass for different size blocks were calculated using finite element techniques and are documented in *Rock Fall on Drip Shield* (BSC 2001l, Section 5.2 and Table 7-1). Preliminary results from the analysis indicated that the impact would not dent the drip shield in such a way that it would contact the waste package. (Design criteria are presented in *Emplacement Drift System Description Document* [CRWMS M&O 2000ab].) The impact from a 10-metric-ton block was estimated to produce one 13-cm (5-in.) long crack in a 3-m (10-ft) long portion of a drip shield segment because of stress corrosion cracking that could occur after the rockfall (BSC 2001l, Table 6-1). Smaller rocks, such as a 2-metric-ton rock, were estimated not to produce enough residual stress to initiate stress corrosion cracking. It is expected that such stress corrosion cracks would be narrow and would not conduct much water flow (see Section 4.2.4). The calculation is conservative because it does not take credit for energy expended by fracturing of the rock or dislocation of the drip shield.

Effects from rockfall events involving multiple rock blocks have not been analyzed explicitly. However, because the dimensions of the maximum expected block size are of the order of the dimensions of the waste packages, it is reasonable to assume that multiple falls of blocks of the maximum size would have to act independently. The effects from multiple, smaller-size block falls would be bounded by the analyses of the effects of the maximum block size.

4.2.3.3.6 Limitations and Uncertainties

As discussed in Section 4.4.1.2 of this report, uncertainties are an inherent component of the TSPA method. Uncertainty is introduced through the conceptual model selected to characterize a process, as well as the mathematical, numerical, and computational approaches used to implement the model. Uncertainty is also introduced from imperfect knowledge of important parameters used for input to the models (e.g., physical properties). This section emphasizes limitations and uncertainties relative to the in-drift physical and chemical environment: (1) the thermal-hydrologic-chemical model used to characterize seepage water chemistry that enters the drift, (2) the in-drift chemical environment model and supporting analyses, and (3) the rockfall model and supporting analyses.

Since the TSPA-SR model, the DOE has performed several supplemental activities to address uncertainties and limitations in the TSPA-SR model. Additionally, as noted in Section 4.1.4, the DOE is evaluating the possibility for mitigating uncertainties in modeling long-term repository performance by operating the design described in this report at lower temperatures. Consequently, some of the models describing the thermal-hydrologic-chemical model, precipitates salts model, and the drift degradation model have undergone further evaluation since the TSPA-SR model. Some alternative models have been implemented and sensitivity analyses conducted to address parameter and model uncertainties. These supplemental analyses are summarized in *FY01 Supplemental Science and Performance Analyses* (BSC 2001a, Sections 4, 5 and 6). The sensitivity of TSPA model results to alternative process models is discussed in Volume 2, Sections 3.2 and 4.2 of *FY01 Supplemental Science and Performance Analyses* (BSC 2001b) and is summarized in Section 4.4.5.5 of this report.

Thermal-Hydrologic-Chemical Seepage Model Limitations and Uncertainties—Uncertainties exist in the thermodynamic and kinetic input data used in the model. For example, as the concentrations of dissolved solutes increase during evaporation, the theoretical limitations of the chemical activity model may be exceeded. Rapid boiling can lead to mineral precipitation that is controlled by nucleation kinetics and other surface-related phenomena. The specific conditions for which the model becomes invalid, however, may not be important for the overall dynamics of the system. Geochemical reactions are a strong function of temperature and the presence of water, both of which are better constrained than the rates of reaction and may control the spatial distribution even if the exact quantities of the phases at a given time are uncertain (CRWMS M&O 2000al, Section 3.3.4).

The model is based on information obtained from thermal testing in the middle nonlithophysal unit of the Topopah Spring Tuff, which may exhibit somewhat different thermal-hydrologic behavior or mineralogy than lower lithophysal units, in which most of the repository emplacement drifts would be located. Although this could change the system response, it is noted that the bulk chemistry is similar for all the welded host rock units (CRWMS M&O 2000al, Section 3.3.4). Thermal testing that is planned for the lower lithophysal unit will evaluate the applicability of the current model over the repository footprint.

Another aspect of thermal-hydrologic response that will affect aqueous and gas-phase chemistry in the host rock is buoyant gas-phase convection (CRWMS M&O 2000cm), controlled by the large-scale permeability. As discussed previously, gas-phase convection will be an important source of carbon dioxide and oxygen as chemical reactants to the in-drift chemical environment. Buoyant gas-phase convection is not evident from the Drift Scale Test, probably because the rock bulk permeability at this location does not support it. However, results from the unsaturated zone flow model (Section 4.2.1) indicate that permeability of the host rock increases with scale, and current thermal-hydrologic models do not incorporate mass transfer along the axes of the drift openings. Therefore, it is likely that further investigation will show that gas-phase convection in the potential repository will exceed that observed in the Drift Scale Test. It is anticipated that the magnitude of gas phase convection will be great enough to supply sufficient amounts of gas through drift openings to preclude depletion of gas components through chemical reactions with drift components (CRWMS M&O 2000cg, Sections 6.3.2 and 6.3.3).

Section 4.2.2.3.5 summarized supplemental studies to the TSPA-SR model related to physical changes in permeability and seepage resulting from thermal-hydrologic-chemical processes. These studies also addressed thermal-hydrologic-chemical model uncertainties related to the chemistry of potential seepage water. Specific studies included:

- Supplemental sensitivity studies of different initial water and gas boundary conditions (BSC 2001a, Section 4.3.6.5)
- Simulated evolution of water and gas compositions in the Tptpmn and Tptpll units (BSC 2001a, Section 6.3.1.4.3)
- Modified base-case and extended case geochemical systems (BSC 2001a, Sections 4.3.5.3.2, 4.3.6.4, and 6.3.1.5).

These activities included a range of different input data and assumptions, including thermodynamic and kinetic data input data (BSC 2001a, Sections 4.3.6.4 and 6.3.1.4).

Precipitates and Salts Model Limitations and Uncertainties—This modeling approach is based on literature data that describe the minerals and salts produced by evaporative concentration and the relations between solution composition and relative humidity. In certain aspects, the thermal-chemical data support is incomplete. Therefore, the accuracy of this model was tested using independent collected laboratory data for the evolution of solids and water composition during evaporation. As described in *In-Drift Precipitates/Salts Analysis* (CRWMS M&O 2000cl, Section 7.3), the precipitates and salts model is expected to provide results that are within an order of magnitude for chloride concentrations and ionic strength and within a pH unit for pH predictions. This degree of accuracy is acceptable because it greatly reduces the potential ranges of these variables, thereby considerably reducing uncertainty.

Data were not available to directly evaluate the accuracy of the low-relative-humidity salts model.

The model did, however, produce reasonable trends and results in chloride and ionic strength outputs in its applied relative humidity range and produces consistent results at 85 percent relative humidity, where the high-relative-humidity salts model takes over (CRWMS M&O 2000cl, Section 7.3).

Simplifying assumptions were required to reduce the complexity of the precipitates and salts analysis and to avoid sophisticated approaches where data were lacking, although these assumptions tended to be conservative. The greatest uncertainties in the analysis are likely the thermal-hydrologic and thermal-hydrologic-chemical predictions and other predicted inputs to the analysis (CRWMS M&O 2000cl, Section 7.3). Therefore, the models were applied for a variety of these conditions.

The precipitates/salts model has been modified in several ways since the TSPA-SR model analyses. Each modification involved the high relative humidity submodel. The Pitzer database was improved by the addition of several minerals and thermodynamic data, and the amount of output data reported in lookup tables was increased (BSC 2001a, Section 6.3.3.4).

Additional discussion of uncertainties related to the precipitate and salts model is described in supplemental studies (BSC 2001a, Sections 6.3.3.3, 6.3.3.4, and 6.3.3.5). Supplemental studies emphasized selected uncertainties, including the sensitivity of starting water composition on evaporative chemical evolution and effects of mineral suppression (BSC 2001a, Section 6.3.3.5.1). Sensitivity studies show in-drift chemistry to be sensitive to starting water composition and that thermodynamic and kinetic data are secondary in importance or negligible (BSC 2001a, Section 6.3.3.5). These studies also show that using the water composition obtained from the thermal-hydrologic-chemical model is reasonable, as implemented in the TSPA-SR model and supplemental TSPA model analyses.

Microbial Communities Model Limitations and Uncertainties—This model is not intended to quantify localized microbial activity or its consequences but bounds overall microbial growth and activity in the engineered barrier system. It has been validated by testing against laboratory data, natural system observations, and other modeling efforts, as described in Section 6.6 of *In-Drift Microbial Communities* (CRWMS M&O 2000cp). Comparison with these independent data sets indicates that the estimates are within an order of magnitude of the actual values.

The approach uses a well-mixed reaction system to represent the emplacement drift and provides estimates of total biomass production that can be used to bound the extent of microbially influenced corrosion of the waste package. In this approach, one of the primary uncertainties is in the degradation rates that supply nutrients and energy for microbial growth. This is evaluated by varying the rates over large ranges and using bounding results (CRWMS M&O 2000cp, Section 6).

Engineered Materials Effects Modeling Limitations and Uncertainties—The rate of steel corrosion for sub-oxic conditions, including the effects of microbial activity, is an important factor in predicting the oxygen budget in the emplacement drifts. Current estimates for steel corrosion are based on (1) abiotic test results obtained for similar steel under oxic conditions and (2) preliminary data for microbially influenced corrosion of similar steel at water-saturated and nutrient-augmented culture conditions. The results for oxic conditions overestimate the rate of oxygen consumption for conditions of decreased oxygen availability, which could occur for a few hundred years in the repository during peak thermal conditions. Applicability of the available microbial testing data to environmental conditions in the repository is more uncertain (CRWMS M&O 2000cg, Section 6.3).

Boiling of water during the thermal event will produce water vapor that will displace much of the air from the drift, with the result that oxygen will be depleted. This may lead to decreased corrosion rates, but the extent of such decreases is uncertain for steel and corrosion-resistant materials such as titanium and Alloy 22. In any case, the effect of decreased oxygen availability will be of limited duration.

Supporting analyses to the TSPA model has previously demonstrated that including these uncertainties would increase the potential for reduced corrosion and solubility, which would have a beneficial impact on performance (BSC 2001a, Section 6.3.2.3.1).

Conceptualization of leachate that could be contributed from degradation of cement grout is adapted from simplifying assumptions and studies of concrete reported in the literature (CRWMS M&O 2000cg, Section 6.3.1; CRWMS M&O 2000as, Section 3.1.2.3.5). Confirmatory testing of rock bolt longevity, carbonation of the grout, microbial attack of organic superplasticizers, and other aspects of grouted rock bolt performance has not been undertaken. The final design of ground support in the emplacement drifts is under development, and analysis of ground support function is preliminary. Accordingly, the longevity of grouted rock bolts in response to thermal loading and environmental conditions remains somewhat uncertain. Rock-mass deformation could lead to failure of the rock bolts (not necessarily associated with failure of the drift openings).

Supporting the TSPA-SR model analyses, supplemental analyses have provided additional confirmation indicating cement leachate-influenced seepage water would have a negligible affect on in-drift chemistry (BSC 2001a, Section 6.3.2.3.2).

Limitations and Uncertainties on Conditions Used to Model Barrier Corrosion—Microbial activity on the waste package surface under an intact drip shield may be negligible, even above 90 percent relative humidity, as long as water has not leaked through the drip shield onto the waste package and the waste package has not directly contacted the invert. Thus, significant corrosion would not commence until the drip shield fails and water contacts the waste package. Similarly, if salt-tolerant organisms are present, the relative humidity threshold for microbially influenced corrosion may decrease to 75 percent, which would mean that the onset of microbially influenced corrosion could shift to an earlier time. Such a shift represents only a small fraction of the time that microbial processes are modeled to be present. Furthermore, uncertainty as to the timing for the onset of general corrosion or microbially influenced corrosion is of low importance for performance assessment because the expected corrosion rate for the waste package, even with microbes present, is low enough that a shift in the timing of the onset of corrosion is insignificant to the overall performance of the potential repository. Further discussion of corrosion rates for the drip shield and waste package is provided in Section 4.2.4.

Common scale minerals that are produced from natural waters include calcite, gypsum, and silica (CRWMS M&O 2000ck, Section 6.1.1). If seepage occurs, the chemical components of these minerals will be present in waters that contact the drip shield and waste package. The tendency for scale formation is enhanced by evaporative concentration and changes in pH. Scale can protect the underlying material if it forms a dense adherent layer, but it may have a deleterious effect if it forms a porous layer or a crevice with the underlying material. Interfaces between scale-covered and bare regions of the surfaces might be subject to corrosion. Few data on the effects of scale are presently available, but related laboratory tests have been performed to evaluate the potential for crevice corrosion. The results show that crevice corrosion is insignificant for titanium and Alloy 22 at the expected repository temperature and humidity. By inference, the effects of scale are also thought to be insignificant.

Another potentially important aspect of scale formation is the production of decomposition products, such as lime, from scale minerals at elevated temperatures. Subsequent dissolution of such products by seepage water or deliquescence could produce highly alkaline solutions. Decomposition temperatures for potential scale minerals are known, and some are within the operating temperature limits for the waste package (CRWMS M&O 2000ck, Sections 4.1.11 and 6.11). However, as discussed previously, the presence of gaseous carbon dioxide in the drift environment implies that the formation of highly alkaline hydroxide species is unlikely.

Rockfall Model Limitations and Uncertainties—The usefulness of the rockfall model is affected by how well the data inputs describe the actual fracture conditions. The natural variability of fractures within a rock mass always represents uncertainty in the design of structures in rock. The extensive fracture data collected at Yucca Mountain provide a good representation of fracturing at the emplacement drift horizon. The range of fracture variability from tunnel mapping has been captured in the rockfall model through multiple Monte Carlo simulations of the rock mass. To account for uncertainties associated with seismic, thermal, and time-dependent effects on rockfall, a conservative reduction of joint strength parameters has been included in the approach (CRWMS M&O 2000e, Section 5).

Sensitivity analyses supplemental to the TSPA-SR model did not change the results of the rockfall model analyses (BSC 2001a, Section 6.3.4.9). Consequently, the process remains insignificant to performance and remains screened from TSPA analyses (BSC 2001a, Section 6.3.4.6).

4.2.3.3.7 Alternative Conceptual Processes

As with limitations and uncertainties, some of the following alternative conceptual models have been addressed in supplemental analyses and summarized in *FY01 Supplemental Science and Performance Analyses* (BSC 2001a, Section 1; BSC 2001b, Section 1).

Alternative Concepts for Thermal-Hydrologic-Chemical Seepage Model—Alternative approaches for modeling the compositions of the gas-phase and liquid seepage have been evaluated in *Engineered Barrier System: Physical and Chemical Environment Model* (CRWMS M&O 2000cg, Sections 6.2 and 6.7). Both the bicarbonate-type and chloride-sulfate-type waters were evaluated for a range of carbon dioxide conditions. The results were used to evaluate the carbon dioxide budget, taking into account processes in the host rock and within the drifts, as discussed previously. The liquid and gas compositions obtained are comparable to results from the thermal-hydrologic-chemical seepage model, which were abstracted for the TSPA-SR model.

As noted in Section 4.2.2.3.5, supplemental studies have evaluated a number of additional alternative starting water compositions in sensitivity analyses. Additional water compositions included water perched on top of the Calico Hills formation, water collected from the Drift Scale and Single Heater Tests, and water predicted by the thermal-hydrologic-chemical model, as well as other seepage water compositions discussed in this section (BSC 2001a, Section 6.3.3.5). Alternative conceptual models described in Sections 4.2.2.3.5 and 4.2.3.3.6 include alternative initial water and gas compositions, alternative host rock assumptions, and modified base-case and extended case geochemical systems (BSC 2001a, Sections 4.3.5.3.2, 4.3.6.4, 4.3.6.5, 6.3.1.4.3, and 6.3.1.5). In general, the sensitivity studies suggest that the models incorporated in the TSPA-SR are reasonable or conservative.

Alternative Concepts for Precipitates and Salts Model—An alternative approach for representing the composition of waters contacting the drip shield and waste package would be a bounding concept. Considering that some dripping of water onto the drip shields may occur throughout the repository in small quantities because of condensation, small accumulations of minerals and salts, on the scale of individual droplets, could occur in locations where seepage will never occur. Microscopic quantities of salts would interact with changes in the relative humidity but would not be mobilized by flow or diluted by seepage. In this alternative bounding approach, the environment on the drip shield surface would be represented by the permanent presence of minerals and soluble salts or the solutions obtained when they equilibrate with water vapor in the air (CRWMS M&O 2000cg). Although simpler than the current precipitates and salts model used for TSPA-SR, this approach would not yield very different corrosion conditions. Current estimates of corrosion rates are small, with limited sensitivity to the presence of soluble salts (see Section 4.2.4).

An alternative model for seepage/invert interactions has been developed but has not yet been implemented in its entirety (BSC 2001a, Section 6.3.3.4.2.1). This alternative model abstracts in-drift mixed solutions using ionic strength, pH, and an acid neutralizing capacity parameter (which is an indication of the resistance of a solution to pH changes). The abstracted solutions are mixtures of seepage fluxes from the crown above the drift, the water wicked through the rock and corroded metals in the invert, and the diffusion film or flux from a waste package after failure.

Alternative Concepts for Microbial Communities Model—As stated previously, the implemented model bounds the overall production of biomass in the emplacement drifts. Two approaches, while not precisely alternatives to the microbial communities model, could be used to extend the model from estimation of biomass to estimation of bounding rates for microbially influenced corrosion. The first approach is an empirical approach based directly on microbial corrosion laboratory test data. The second approach, which is the principal alternative concept for predicting microbial effects on the bulk chemical environment, is the chemical kinetics approach mentioned previously. In this concept, biotic and abiotic chemical reactions are treated similarly, as quantitatively explicit reactions distinguished by different reaction rates. Reaction pathways would include organic species and compounds produced by microbial activity. This approach has long been recognized as an alternative but has not been used because reasonable data support is not available. The advantages of the approach would include quantitative predictions involving specified chemical systems. Pathways for microbially mediated reactions can be complex, and extensive laboratory testing could be required to represent conditions in the repository. Process models for these approaches have not been developed.

Alternative Concepts for Engineered Materials Effects Modeling—An alternative concept for the possible effect of steel on the performance of the titanium drip shield was analyzed. Specifically, the potential for hydrogen embrittlement and cracking of the titanium was evaluated. It is likely that steel ground support members will eventually fail from corrosion, possibly augmented by rock support loads, and fall onto the drip shields so that steel would come to rest on the titanium. This concept is neglected in the TSPA-SR model because (1) at the time of failure the steel will probably be coated with oxides that have no deleterious effect on titanium and (2) fine cracks in the drip shields will not transmit significant amounts of water (CRWMS M&O 2001c, Section 6.1), similar to stress corrosion cracks in the waste package (see Section 4.2.4).

Alternative Approaches for Modeling Rockfall—An alternative approach that was considered for modeling rockfall involved the use of multidimensional distinct-element analysis (CRWMS M&O 2000e). The approach has the benefit of directly applying dynamic loading to the rock mass. However, the approach is deterministic and cannot readily accommodate the available data on variability of fracturing in the potential host rock units. Accordingly, distinct element modeling was used only to confirm results obtained with the probabilistic key-block analysis and to assess thermal effects on host rock permeability (see Section 4.2.2.3.4).

4.2.3.3.8 Model Calibration and Validation

Thermal-Hydrologic-Chemical Seepage Model Calibration and Validation—The goal of model validation is to determine reasonable bounds on the system behavior over 10,000 years or longer, based on relatively short-term tests. The thermal-hydrologic-chemical Drift Scale Test model is an implementation of the repository-scale thermal-hydrologic-chemical seepage model for the situation of the Drift Scale Test. The results were compared to gas and water samples, representing potential seepage collected during the Drift Scale Test (CRWMS M&O 2000al, Section 3.6.3.2) as a means to validate the repository scale model. These comparisons include gas-phase carbon dioxide concentrations as a function of time and space, the pH of waters collected in boreholes, and general observations on changes in concentrations of chloride and other aqueous species.

Gas-phase carbon dioxide concentrations in the model results and in the measured values showed a similar halo of strongly elevated values (approximately 2 orders magnitude greater than the air in the observation drift) around the Drift Scale Test heaters that grew outward over time. Modeled pH values of fracture waters in the drainage zones of around 6.5 to 7.5 (calcite–silica–gypsum system) are within one pH unit of waters collected from boreholes during the Drift Scale Test. Increases in the modeled pH of the waters as the rock around the boreholes heated further and began to dry out were also similar to the measured values where multiple samples were collected over time. This indicates that the model also captured the time-dependence of thermal-hydrologic-chemical processes. Simulations employing a more complex set of minerals and aqueous species estimate pH values about 0.5 to 1 pH unit higher than for the calcite–silica system. Such behavior may be more characteristic of longer time-scale water–rock interaction, which can be validated as the Drift Scale Test produces data that reflect conditions of more stable isotherms, as opposed to the data that were collected during the more transient first two years of the heating phase.

Concomitant increases (with pH and temperature) in measured silica concentrations and depletions in calcium suggest silicate mineral dissolution and calcite precipitation, trends that were also predicted by the model. Ongoing studies (by sidewall sampling and overcoring) of the actual minerals precipitated in fractures and their effect on hydrologic properties will allow for further comparisons to model results.

Measured chloride concentrations (a conservative species that shows the effects of dilution, boiling, and fracture–matrix interaction) are 5 to 10 times lower than in the pore water, a characteristic that was also captured by the model in the drainage zones. This validates that the model approximates fairly well the overall effects of dilution through condensate formation and fracture–matrix interaction (diffusive equilibration).

Precipitates and Salts Model Calibration and Validation—The normative precipitates and salts model approach (CRWMS M&O 2000cg, Section 6.5) was applied to the laboratory test results on a qualitative basis, and the results were in reasonable agreement for the bicarbonate-type water. There evidently is some sensitivity to the relative availability of calcium and sodium to form sulfate salts, which is not accounted for in the model. Minor species such as sylvite were identified by the normative model but were not detected in the laboratory tests because they were scarce and because of interference from ambient humidity. Additional testing with the chloride-sulfate-type water produced similar agreement between the normative assemblage and the minerals observed on complete evaporation. From these results, the normative model is determined to provide a valid approximation to the major minerals and salts formed on complete evaporation of waters with composition similar to either J-13 water or matrix pore water.

The low- and high-relative-humidity salts models were independently developed and validated with laboratory data (CRWMS M&O 2000cl, Section 4.1.2). The low-relative-humidity salts model approach is conservative because it tends to shorten the dry period by not allowing dry conditions for relative humidity greater than 50 percent in the presence of nitrate salts. Also, it predicts elevated chloride concentrations at low relative humidity (CRWMS M&O 2000cl, Section 7.1). The model is valid because it reproduces trends in the known behavior of salts and provides results that are within an order of magnitude of independently developed data. Such accuracy reduces uncertainty associated with the processes that control water composition at low relative humidity. The low-relative-humidity salts model results that are important for TSPA modeling are a decrease in ionic strength (due to the thicker water film) and an increase in chloride concentration as the relative humidity rises from 50 to 85 percent.

Validation of the high-relative-humidity salts model is approached using results from laboratory tests, including those described previously in which bicarbonate-type and chloride-sulfate-type waters were evaporated, and handbook solubility values for pure salts. Reasonable agreement is obtained between measured and modeled values for pH and the concentrations of sodium, carbonate species, fluoride, chloride, and sulfate (CRWMS M&O 2000cl, Section 6.5.1). Agreement to within an order of magnitude is obtained for other constituents, which is acceptable for use in abstracted models for the TSPA. As an additional check, the model is also used to calculate the solubilities of several sodium and potassium salts that are potentially important products of evaporating J-13 water.

Calculated values are within a factor of 2 of the handbook values, up to 10 molal (the limit of the Pitzer model).

Microbial Communities Model Calibration and Validation—This is a bounding model that has been validated by comparison to laboratory and field data. Both model validation and code verification are described in Section 6.6 of *In-Drift Microbial Communities* (CRWMS M&O 2000cp). In these applications, agreement was obtained with observed microbial abundances within the order-of-magnitude tolerance level identified for the use of this model. Three comparisons were used:

- Replication of model results originally calculated for the Swiss repository program demonstrates that the code used for the microbial model (MING) functions correctly where natural materials are combined with engineered materials.
- Modeling of microbial conditions investigated underground at Yucca Mountain and at an analogue site at Rainier Mesa replicated the ambient microbial abundance to within an order of magnitude and confirmed that water and phosphorous availability are limiting factors to microbial growth.
- Modeling of the laboratory tests shows that the numbers of organisms calculated by MING can agree to within an order of magnitude with independently measured data from both energy-limited and nutrient-limited tests.

Engineered Materials Effects Model Calibration and Validation—Models for oxygen consumption by steel corrosion, the effects of cementitious materials, and the impact of ferric-oxide colloids on radionuclide transport are based on bounding approaches, and the best available supporting data are used. Key uncertainties and approaches to confirmation of these bounding arguments have been identified (CRWMS M&O 2000cg, Sections 6.3 and 6.6).

Rockfall Model Calibration and Validation—The rockfall model involved the use of probabilistic key block theory, which is an accepted approach for analyzing this type of geotechnical problem. The static key block results are in agreement with observed key block occurrence in the Exploratory Studies Facility main drift and cross-drift (CRWMS M&O 2000e, Section 7.2). The results from the rockfall model have shown that key blocks are most predominant in the Tptpmn unit, which agrees with field observations. The size of key blocks observed in the field is generally less than one cubic meter, which agrees with the simulated distribution of block sizes.

The seismic component of the rockfall model involves a quasi-static method of reducing the joint strength parameters. This method was verified based on the test runs using the dynamic functions of the distinct element code UDEC. Comparison between results from the dynamic and quasi-static analyses shows a consistent prediction of block failure at the opening roof (CRWMS M&O 2000e, Attachment V).

4.2.3.4 Total System Performance Assessment Abstraction

This section describes abstraction of only those models selected for inclusion in the TSPA. The microbial communities model and the models used to bound the effects of engineered materials are determined to have minor impacts on calculated waste isolation performance (although it is acknowledged that microbially influenced corrosion may affect the longevity of Alloy 22 locally) and are excluded from the base case. Also, design analysis has shown that rockfall will not degrade the functionality of the drip shield or waste packages, so the rockfall model is also not included in TSPA-SR.

Abstraction of the Thermal-Hydrologic-Chemical Seepage Model for the Total System Performance Assessment—The thermal-hydrologic-chemical abstraction using the mean distribution of infiltration rate (CRWMS M&O 2000a, Section 3.3.3.4.2), including climate change, is calculated for both geochemical systems discussed above. The abstracted results for both the less complex and more complex chemical systems are shown in Table 4-17 (CRWMS M&O 2000al,

Table 4-17. Thermal-Hydrologic-Chemical Abstraction for the Mean Infiltration Rate Case with Climate Change

Parameter	Preclosure (Period 1) 0 to 50 years Abstracted Values 80°C	Boiling (Period 2) 50 to1,000 years Abstracted Values 96°C	Transitional Cooldown (Period 3) 1,000 to 2,000 years Abstracted Values 90°C	Extended Cooldown (Period 4)[a] 2,000 to 100,000 years Abstracted Values 50°C
Constituents from the Limited Chemical System (calcite–silica–gypsum)				
log CO_2, vfrac	-2.8	-6.5	-3.0	-2.0
pH	8.2	8.1	7.8	7.3
Ca^{2+}, molal	1.7×10^{-3}	6.4×10^{-4}	1.0×10^{-3}	1.8×10^{-3}
Na^{+}, molal	3.0×10^{-3}	1.4×10^{-3}	2.6×10^{-3}	2.6×10^{-3}
SiO_2, molal	1.5×10^{-3}	1.5×10^{-3}	2.1×10^{-3}	1.2×10^{-3}
Cl^{-}, molal	3.7×10^{-3}	1.8×10^{-3}	3.2×10^{-3}	3.3×10^{-3}
HCO_3^{-}, molal	1.3×10^{-3}	1.9×10^{-4}	3.0×10^{-4}	2.1×10^{-3}
SO_4^{2-}, molal	1.3×10^{-3}	6.6×10^{-4}	1.2×10^{-3}	1.2×10^{-3}
Constituents from the More Complete Chemical System (including aluminosilicates)				
Mg^{2+}, molal	4.0×10^{-6}	3.2×10^{-7}	1.6×10^{-6}	7.8×10^{-6}
K^{+}, molal	5.5×10^{-5}	8.5×10^{-5}	3.1×10^{-4}	1.0×10^{-4}
AlO_2^{-}, molal	1.0×10^{-10}	2.7×10^{-7}	6.8×10^{-8}	2.0×10^{-9}
$HFeO_2^{-}$, molal	1.1×10^{-10}	7.9×10^{-10}	4.1×10^{-10}	2.4×10^{-11}
F^{-}, molal	5.0×10^{-5}	2.5×10^{-5}	4.5×10^{-5}	4.5×10^{-5}

NOTES: [a] Thermal-hydrologic-chemical calculations have been carried out to 100,000 years, while TSPA calculations have been carried out to 1 million years. Source: CRWMS M&O 2000c, Table 3.10-3.

Section 3.3.1). The evolution of chemical conditions at the drift wall is presented as a series of four discrete time periods for the TSPA-SR calculations: (1) preclosure, (2) boiling, (3) transitional cooldown, and (4) extended cooldown. The log carbon dioxide value represents the composition of gas at the drift wall. These time periods are selected so that relatively constant concentrations can be defined for constituents of interest. After the extended cooling period, the system is considered to have returned to the ambient conditions before thermal perturbation. For both chemical systems considered, major differences in concentrations for key constituents (factor of 10) are limited to calcium, sodium, and bicarbonate ions.

Abstraction of the Precipitates and Salts Model for the Total System Performance Assessment—For the TSPA-SR model, the evolution of water in the repository drifts as temperature decreases and relative humidity increases over time is generalized as an evolution from brine to increasingly dilute water. This evolution is modeled as a succession of time intervals. In each interval, the incoming seepage flow and its composition, as well as temperature, are assigned constant values; the evaporation rate varies, and the in-drift chemical environment is determined from the evolution of thermal-hydrologic conditions at the particular location evaluated (CRWMS M&O 2000a, Section 3.3.4).

Below 50 percent relative humidity, any salts present in the drift environment will exist in crystalline form and will not form brines. At relative humidities between 50 and 85 percent, salts in the environment will deliquesce and form brines; compositions are provided by the low-relative-humidity salts model. Above 85 percent relative humidity, all of the salts are considered dissolved, and the composition is estimated by the high-relative-humidity salts model using a quasi-steady-state approximation of the degree of evaporative concentration (CRWMS M&O 2000a, Section 3.3.4.5.1).

For each time interval, values of the temperature, carbon dioxide partial pressure, seepage, and evaporation rate are obtained from other models. Lookup tables are then developed for the in-drift water composition to be used in the TSPA, based on a set of calculations using the low-relative-humidity salts model and the high-relative-humidity salts model. The lookup tables are developed for the following conditions: temperature at 95°, 75°, 45°, and 25°C (203°, 167°, 113°, and 77°F); carbon dioxide partial pressure at 10^{-1}, 10^{-3}, and 10^{-6} atmospheres; and evaporative concentration ranges up to a thousandfold (CRWMS M&O 2000a, Section 3.3.4.5.1).

Inputs to and outputs from the precipitates and salts model were abstracted for use in the TSPA-SR model (CRWMS M&O 2001b, Section 1; CRWMS M&O 2000cg, Section 6.7.4). The abstracted results used in the TSPA-SR model were based on the thermal-hydrologic-chemical model as follows:

- Incoming seepage composition represented by the thermal-hydrologic-chemical abstraction
- Carbon dioxide fugacity and temperature fixed at thermal-hydrologic-chemical abstracted values.

The supplemental TSPA model used a modified abstraction of the thermal-hydrologic-chemical model. Modifications included the effects of operating temperature, the effects of different carbon dioxide partial pressures, and the effects of different initial pore water (and infiltration) compositions (BSC 2001a, Sections 6.3.1.6.3 and 6.3.1.9).

Likewise, the precipitates and salts model abstraction has been updated in supplemental TSPA modeling to include the effect of the concentrations of a revised suite of elements and a select number of aqueous species used to estimate alkalinity (BSC 2001a, Section 6.3.3.6). Another improvement to the precipitates and salts model is consideration of condensation. The combined effect of improvements to the near-field geochemical model shows differences at the subsystem level composition (BSC 2001a). However, supplemental analyses do not show a significant impact at the TSPA level for either higher- or lower-temperature operating modes (BSC 2001b, Sections 3.2.4.2 and 4.2.4).

4.2.4 Waste Package and Drip Shield Degradation

The roles of the waste package and drip shield are discussed in detail in Section 3. This section addresses the expected performance of these components in the potential repository and, along with Sections 4.2.1 through 4.2.6, provides an explanation of the relationship of the waste package and the geologic environment at Yucca Mountain.

The degradation process models and the abstracted models discussed in this section serve as feeds to the WAPDEG code, which integrates the various models to address the overall performance (degradation rates) of the waste package and the drip shield. WAPDEG results, in turn, are used as feeds to the overall TSPA-SR. Specifically, the integrated model included in the WAPDEG performance assessment code used repository environmental conditions as a function of time from other process models to estimate the performance of the waste package and drip shield in terms of time to failure.

As noted in Section 4.1.4, the DOE is evaluating operation of the repository at lower temperatures. The conceptual basis and model abstractions presented in this section reflect the effects of higher-temperature operating modes, specifically those implemented in *Total System Performance Assessment for the Site Recommendation* (CRWMS M&O 2000a, Section 3.4). Alternative thermal operating modes and/or conservatisms and conceptual uncertainties have been reevaluated since the TSPA-SR model and are reported or summarized in *FY01 Supplemental Science and Performance Analyses* (BSC 2001a, Section 9; BSC 2001b, Sections 3 and 4).

4.2.4.1 Conceptual Basis

Lifetimes of the drip shield and waste package depend on the environmental conditions to which they are exposed and the degradation processes that occur in that environment. Section 4.2.3 describes the conceptual understanding of the evolution of physical and chemical conditions in the repository emplacement drifts, the models used to represent those conditions, and the experimental data that support and contribute to the validation of the models. Environmental conditions within the drifts that influence the degradation of the waste package and drip shield are tightly coupled to the thermal-hydrologic and geochemical processes occurring in the rock surrounding the drifts. These processes involve the vaporization and condensation of water under changing thermal conditions, redistribution and precipitation of dissolved salts, and the effects of gaseous species on solution chemistry. Included in the conceptualization are the contributions of construction material degradation processes (i.e., rock structural support materials and cementitious grout) and the effects of microbial action.

Once the exposure environments have been established, the most important and relevant degradation processes can be identified, which in turn can be used for selecting engineered materials for the drip shield and the waste package. This section discusses the degradation modes of the waste package and drip shield materials under the changing environmental conditions. Corrosion is the degradation process most relevant and important to the selection of the materials for the waste package and drip shield. Mechanical deformation of the waste package and drip shield are estimated to be less significant to the waste package containment time than corrosion (CRWMS M&O 2000n, Section 1.5). A number of corrosion processes have been investigated in detail and the results used to support the selection of materials and the design of these components.

Waste Package and Drip Shield Materials—Degradation modes for the drip shield and waste package are dependent on the materials used in these components and as mentioned earlier, on the environment in which they function. Performance of these materials are reviewed in *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (CRWMS M&O 2000cq) and *General Corrosion and Localized Corrosion of the Drip Shield* (CRWMS M&O 2000cr). Titanium alloys were selected for construction of the drip shield because of their high resistance to corrosion. This corrosion resistance is due to the formation of a passive oxide film, which is stable over a relatively wide range of environments. The rates of general corrosion and dry oxidation (or dry-air oxidation) of this material have been shown to be very low (CRWMS M&O 2000n, Sections 3.1.1.1, 3.1.5.1, and 3.1.5.4).

Alloy 22 (UNS N06022) was selected for construction of the waste package outer barrier. The main alloying elements of this material are nickel, chromium, molybdenum, iron, tungsten, and cobalt. Alloy 22 is less susceptible to localized corrosion in environments that contain chloride ions than Alloys 825 and 625, materials of choice in earlier waste package designs (CRWMS M&O 2000n, Section 3.1.1.2). This material is one of the most corrosion-resistant nickel alloys for the expected range of repository environments (Gdowski 1991, Section 1.2.5). Alloy 22 and its predecessor alloys have been in use for the past 50 years in a variety of environments and have performed extremely well. Figure 4-79 shows the appearance of a test coupon made from Alloy C, which is a predecessor of Alloy 22, after almost 60 years of exposure to a marine environment. Its shiny, mirror-like appearance was restored by rinsing the dirt and sand from the surface. In comparison to Alloy C and C-4, Alloy 22 has greater corrosion resistance. This is based on the fact that Alloy C-4 and Alloy C-276 have a comparable corrosion resistance (Gdowski 1991, Section 1.2.4), and resistance of Alloy 22 to crevice corrosion is greater than Alloy C-276 (Gdowski 1991, Tables 22 and 25).

Stainless Steel Type 316NG will be used for construction of the structural support container inside the waste package outer barrier to increase the overall strength of the waste package. This material is less susceptible to localized corrosion in environments that contain chloride ions than stainless steel 304, but it is more susceptible than other corrosion-resistant materials such as Alloys 22, 625 and 825, which were considered in various waste package designs (CRWMS M&O 2000n, Section 3.1.1.3). However, the stainless steel layer is used primarily for structural support for the outer barrier and not as a corrosion barrier to the ingress of water into the waste package. The key factor in placing the structural material on the inside is that its strength does not begin to degrade until the outer shell is breached by corrosion or other degradation modes. This is in contrast to the VA design

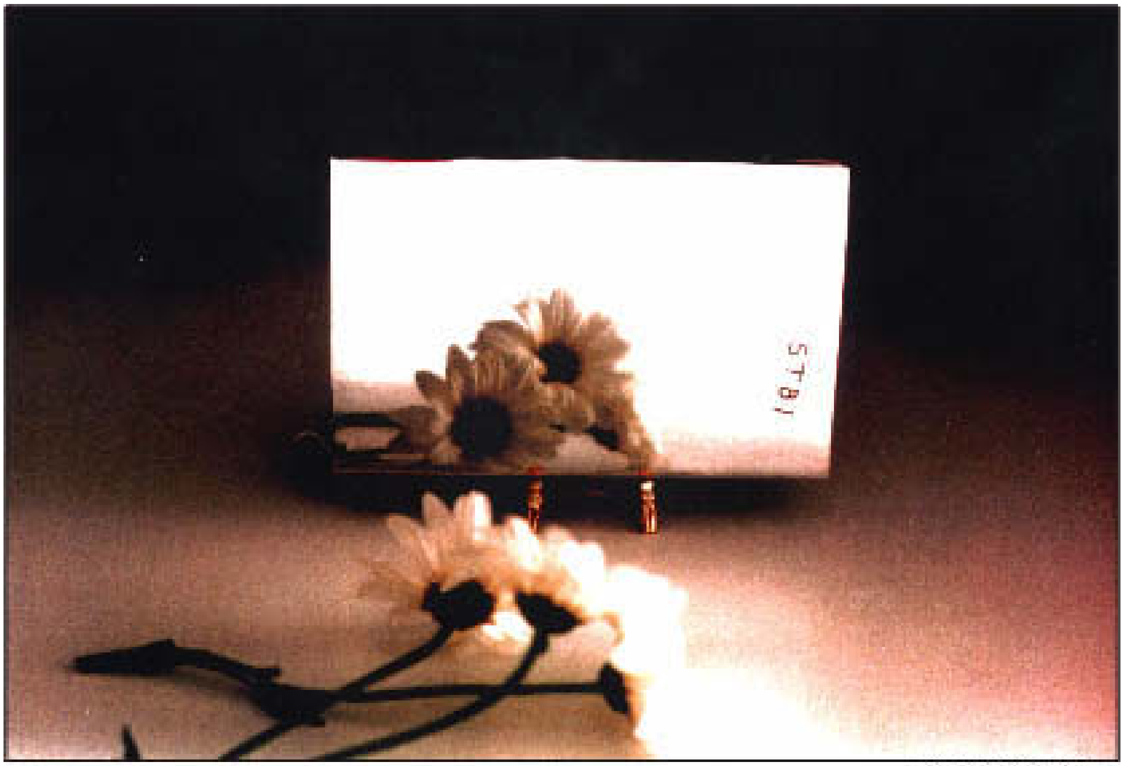

Figure 4-79. Alloy C Test Coupon after Almost 60 Years of Exposure to a Marine Environment
This test coupon has maintained its mirror finish even after 56 years of exposure to a saltwater atmosphere at the Kure Beach (North Carolina) Marine Atmosphere Test Lot. The coupon was cleaned by simply rinsing it with water.

in which the structural carbon steel was the outer shell, with degradation of strength beginning soon after repository closure.

Figures 4-80 and 4-81 provide a visual perspective to illustrate the physical arrangement of the waste packages and the drip shield within the drift. Figure 4-80 shows schematically the arrangement of different types of waste packages and drip shield. Figure 4-81 shows a schematic sketch of a typical waste package designed for 21 pressurized water reactor fuel assemblies, along with the materials used for the various components.

The dual-barrier design of the waste package and the number of options for the thermal design of the potential repository required a comprehensive testing program to evaluate how materials would perform under the wide range of possible conditions in the potential repository.

Degradation processes evaluated for the drip shield and the waste package include general and localized corrosion under humid air and aqueous conditions, stress corrosion cracking, and hydrogen-induced cracking. The effects of microbially influenced corrosion and aging of the waste package outer barrier were also included in the modeling. An integrated model was developed to evaluate the combined effects of the various degradation modes and was used to estimate the range of lifetimes of the drip shields and the waste packages, including an evaluation of uncertainties.

4.2.4.2 Summary State of Knowledge

Surface Environment—The starting waters present at Yucca Mountain are classified into two types: (1) bicarbonate-type water (e.g., J-13 water) and (2) unsaturated zone pore water (chloride-sulfate water). Chemical modeling and laboratory testing of these water compositions have shown that the bicarbonate-type water evolves by evapo-