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9-2		<p>Citation update (Correct DIRS as appropriate)</p> <p>Section 9.1, replace reference (169856) with reference (172463), change:</p> <p><i>BSC 2004. Drift Scale THC Seepage Model. MDL-NBS-HS-000001 Rev 03. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20041111.0001</i></p> <p>To</p> <p><i>BSC 2004. Drift Scale THC Seepage Model. MDL-NBS-HS-000001 Rev 03. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20041201.0008</i></p> <p>This error was identified in CR 4643</p>									

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1. PURPOSE

The purpose of this report is to describe the evolution of the physical and chemical environmental conditions within the waste emplacement drifts of the repository, including the drip shield and waste package surfaces. The abstraction model is used in the total system performance assessment for the license application (TSPA LA) to assess the performance of the engineered barrier system and the waste form.

This report develops and documents a set of these abstraction-level models that describe the engineered barrier system physical and chemical environment. Where possible, these models use information directly from other reports as input, which promotes integration among process models used for TSPA-LA. Specific tasks and activities of modeling the physical and chemical environment are included in *Technical Work Plan for: Near-Field Environment and Transport In-Drift Geochemistry Model Report Integration* (BSC 2004 [DIRS 171156], Section 1.2.2). As described in the technical work plan, the development of this report is coordinated with the development of other engineered barrier system reports.

1.1 INTENDED MODEL USE

The principal intentions for the use of this model and analysis are to:

- Evaluate the evolution of in-drift chemical environments that affect drip shield and waste package durability, and control solubility and colloidal stability of radionuclides in the invert
- Provide inputs, in the form of lookup tables, to total system performance assessment for the license application (TSPA LA) to enable quantification of ionic strength, chloride and nitrate concentration, and pH as functions of relative humidity (RH), $p\text{CO}_2$, and temperature.

This is accomplished through use of the physical and chemical environment models that consist of: seepage evaporation abstraction, dust deliquescence abstraction, and gas abstraction models.

1.2 SCOPE OF MODELS

This report focuses on abstractions of seepage and gas inflow values, based on inputs from the outputs of *Drift-Scale THC Seepage Model* (BSC 2004 [DIRS 172463]) and *Post-Processing Analysis for THC Seepage* (BSC 2004 [DIRS 169858]). This report then predicts in-drift aqueous solution compositions due to seepage and deliquescence of dust using the model developed in *In-Drift Precipitates/Salts Model* (BSC 2004 [DIRS 169863]).

As seepage waters percolate into the drift, their chemical compositions change by evaporation and mineral precipitation. Under higher temperature conditions when seepage does not occur, deliquescence of salts in dust controls the in-drift water chemistry. Evaporation causes dissolved aqueous species concentrations to increase, minerals to precipitate, and the most-soluble components to become concentrated in the resulting solution (brine).

is 982 kg/m; excluded is 75 kg/m, determined from weights listed for committed materials (BSC 2004 [DIRS 169776]).

(Tables 4.1-3 through 4.1-9 intentionally deleted.)

Table 4.1-10. Low-Alloy or Carbon Emplacement Drift Steel Materials and Size Specifications

Component	Material Conformance ASTM Manual	Type of Material	Size Specifications
Gantry Rails	Carbon Steel Type A759 ¹	Carbon Steel Crane Rails	135 lb/yd
Rail Runway Beams with Stiffeners	Carbon Steel Type A588, Grade 50 ²	High-Strength Low-Alloy Steel	W8 × 67
Runway Beam Cap Plates	Carbon Steel Type A588, Grade 50 ²	High-Strength Low-Alloy Steel	PL 1" × 12"
Longitudinal Support Beams	Carbon Steel Type A588, Grade 50 ²	High-Strength Low-Alloy Steel	W12 × 35
Transverse Beams with Stiffeners	Carbon Steel Type A588, Grade 50 ²	High-Strength Low-Alloy Steel	W12 × 72
Stub Column	Carbon Steel Type A588, Grade 52 ²	High-Strength Low-Alloy Steel	W8 × 67
Base Plates	Carbon Steel Type A588, Grade 50 ²	High-Strength Low-Alloy Steel	PL 1" × 12" × 24"

Sources: Material ASTM and size specifications indicated in BSC 2004 [DIRS 169776].

¹ASTM A 759-00 2001 [DIRS 159971], Table 1.

²ASTM A 588/A588M-01 2001 [DIRS 162724], Table 1.

Additional references are necessary to define components that are not plate structures (abbreviated "PL" in Table 4.1-10). The 135-lb/yd gantry rails are defined in *Manual of Steel Construction, Allowable Stress Design* (AISC 1989 [DIRS 107536], p. 1-113); the "W" size specifications are defined in the same reference in the tables on pp. 1-28 and 1-32.

4.1.3 Water and Gas Compositions

THC Seepage—The seepage water compositions used in the seepage evaporation abstraction and their associated equilibrium CO₂ fugacity values are listed in DTN: LB0302DSCPTHCS.002 [DIRS 161976]. This DTN consists of five complete drift scale seepage coupled thermal-hydrological-chemical (THC) modeling results, each representing a different starting porewater as described in *Drift-Scale THC Seepage Model* (BSC 2004 [DIRS 172463]). The THC seepage model output for each water is in Microsoft Excel spreadsheet format:

- CS500/12.0-16.7 (*thc6_w7_r.xls*)
- CS2000/16.5 (*thc6_w4_r.xls*)
- CS1000/7.3 (*thc6_w5_r.xls*)
- SD-9/990.4 (*thc6_w6_r.xls*)
- HD-PERM water (*thc6_w0_r.xls*).

These five waters were selected in the source report to represent the spread of available porewater data and to serve as starting water compositions for the drift scale THC seepage

model. The rationale for the initial selection of these five waters is discussed in *Drift-Scale THC Seepage Model* (BSC 2004 [DIRS 172463], Section 6.2.2.1).

Table 4.1-13 lists the THC seepage model outputs used as inputs to the binning analysis in this report (Section 6.6) and identifies these inputs by starting water composition. Throughout the remainder of this report, they will be referred to by their abbreviated water name.

Instructions on how to initially abstract a single time-water sequence from the large set of results is given in *Post-Processing Analysis for THC Seepage* (BSC 2004 [DIRS 169858], Section 6.2.3.3). These instructions supply 368 water compositions. For crown seepage, this report begins with THC fracture waters in the front region, specifically from “index” number four. For invert seepage, this report begins with THC matrix waters in the front region, again from “index” number four. This information begins the further chemical abstraction process in Section 6.6.2.

(Tables 4.1-11 and 4.1-12 intentionally deleted.)

Table 4.1-13. Source Files for Input to Binning Analysis

Abbreviated Water Name	Filename	Starting Water Composition
W0	<i>thc6_w0_r.xls</i>	HD-PERM water (Alcove 5)
W4	<i>thc6_w4_r.xls</i>	Cross-drift water CS2000/16.5
W5	<i>thc6_w5_r.xls</i>	Cross-drift water CS1000/7.3
W6	<i>thc6_w6_r.xls</i>	Borehole water SD-9/990.4
W7	<i>thc6_w7_r.xls</i>	Cross-drift water CS500/12.0-16.7

Source: DTN: LB0302DSCPTHCS.002 [DIRS 161976].

In-Drift Gas—The files shown in Table 4.1-14 are used as inputs for the in-drift carbon dioxide and oxygen gas analyses.

Table 4.1-14. References for Input Gas Chemistry Analyses

Filename	Starting Water Composition
<i>thc6_w0_r.xls</i> <i>thc6_w0_drift_r.xls</i>	HD-PERM water (Alcove 5)
<i>thc6_w4_r.xls</i> <i>thc6_w4_drift_r.xls</i>	Cross-drift water CS2000/16.5
<i>thc6_w5_r.xls</i> <i>thc6_w5_drift_r.xls</i>	Cross-drift water CS1000/7.3
<i>thc6_w6_r.xls</i> <i>thc6_w6_drift_r.xls</i>	Borehole water SD-9/990.4
<i>thc6_w7_r.xls</i> <i>thc6_w7_drift_r.xls</i>	Cross-drift Water CS500/12.0-16.7

Source: DTN: LB0302DSCPTHCS.002 [DIRS 161976].

Gas Flux—The gas flux across the drift wall and into the drift over time is estimated in Section 6.7.1 using output from *Drift-Scale THC Seepage Model* (BSC 2004 [DIRS 172463]), as listed in Table 4.1-15. The complete set of results in the dataset includes gas flux at the base,

Design Specifications—*D&E/PA/C IED Subsurface Facilities Committed Materials* (BSC 2004 [DIRS 169058], Figure 1 and Note 2) contains the relevant dimensional information for the Stainless Steel Type 316L “Bernold” sheets and “Super Swellex” rock bolts that are currently planned for use as in-drift ground support. This relevant dimensional information is presented in Table 4.1-22.

(Table 4.1-21 intentionally deleted.)

Table 4.1-22. Dimensional Information for Stainless Steel Type 316L Sheets and Rock Bolts

Parameter	Value	Source in BSC 2004 [DIRS 169058]
Sheet Thickness	3 mm	Note 2
Rock Bolt Component	10 Bolts/Row 3.0 m long	Figure 1
Rock Bolt Outer Diameter	54 mm	BSC 2003 [DIRS 164101], Table 3 ^a
Rock Bolt Thickness	3 mm	Note 2
Rock Bolt Row Spacing	1.25 m	Figure 1

^a The source for rock bolt outer diameter is BSC 2003 [DIRS 164101], a superseded IED. The outer diameter of the rock bolts is not provided in the revised design data in the superseding IED (BSC 2004 [DIRS 169058]); therefore, the value of 54 mm diameter is retained here and justified for use because of the lack of this information in BSC 2004 [DIRS 169058].

The material composition of both the Bernold sheets and the rock bolts is contained within ASTM A 276-03 2003 ([DIRS 165006], Section 4.3.2) as indicated on *D&E/PA/C IED Subsurface Facilities Committed Materials* (BSC 2004 [DIRS 169058], Note 4); this is a Stainless Steel Type 316L.

Condition Parameters—The abstracted calculation for Stainless Steel Type 316L corrosion is performed in Sections 6.8.3 and 6.8.4. Table 4.1-23 summarizes the specific inputs utilized to abstract the degree of corrosion as a function of time.

Infiltration Rates—Infiltration rates are used as input (see Table 4.1-23) in Section 6.8 to determine how much water per year to react the stainless steel with. These infiltration rate values are justified for use in *Drift-Scale THC Seepage Model* (BSC 2004 [DIRS 172463], Section 4.1.1.2). As that model’s outputs are inputs to this report (particularly DTN: LB0302DSCPTHCS.002 [DIRS 161976]), the same justification applies here for their continued use in this report.

- ASTM G 1-90 (1999) [DIRS 103515], *Standard Practice for Preparing, Cleaning, and Evaluating Corrosion Test Specimens* was used to provide steel density input found on Tables 4.1-16 and 4.1-23.

4.3.3 Level of Accuracy, Precision, and Representativeness of Results

The accuracy, precision, and representativeness of results are provided for by justifying the selection of the input data used, expressing the range of uncertainty and variability of the model and analyses parameters, and indicating the range of applicability for which the results apply. The representativeness of direct inputs the models described in this report, is discussed in Section 4.1. The level of accuracy for predictions of the chemical environment is addressed in Section 6, specifically, equilibrium vs. kinetics (Section 6.5.2), mineral suppression (Section 6.5.5), basis for binning of seepage compositions (Section 6.6), effects from ground support materials (Section 6.8), evaluation of alternative conceptual models (Section 6.11), lookup table interpolation (Section 7.2.2), and other validation issues that pertain to accuracy (Section 7). Numerical precision is not a significant concern for thermochemical modeling of the in-drift environment, although convergence of EQ3/6 runs is addressed in Section 6.5. Uncertainty in model output is addressed and represented explicitly in the feeds to TSPA (Sections 6.12 and 6.15).

4.3.4 Completion Criteria

This work has been performed consistent with *Technical Work Plan: Regulatory Integration Evaluation of Analysis and Model Reports Supporting the TSPA-LA* (BSC 2004f) and fulfills a portion of the Phase 2 work identified in that plan. Completion of this report also partly addresses Condition Reports including CR-1805 (software range of use), CR-1821 (review of errata), CR-2049 (model validation), CR-2050 (model validation), CR-2586 (records roadmaps), and CR-79 (technical information).

4.3.5 Other Requirements

The boundary conditions for this work were established by feeds from related analyses and model documents including *Drift-Scale THC Seepage Model* (BSC 2004 [DIRS 172463]), *Post-Processing Analysis for THC Seepage* (BSC 2004 [DIRS 169858]), and *Multiscale Thermohydrologic Model* (BSC 2004 [DIRS 169565]), and applicable information exchange drawings.

4.4 INPUTS USED FOR MODEL VALIDATION

This section summarizes the indirect inputs used for model validation (Section 7).

4.4.1 THC Seepage Abstraction Validation Inputs

Five complete drift scale seepage THC modeling results, taken from *Drift-Scale THC Seepage Model* (BSC 2004 [DIRS 172463]), represent the sources of seepage water entering the drift (DTN: LB0302DSCPTHCS.002 [DIRS 161976]). Due to the large amount of information contained within this DTN, specific values are not cited here (Table 4.1-13).

4.4.2 Evaporation of Waters to Form Concentrated Brines

To validate the approach for the EBS seepage evaporation model calculations, a classic model presented by Garrels and McKenzie (1967 [DIRS 123636]) for the evaporation of Sierra Nevada spring water is used. The EBS model simulates evaporation and concentration of these waters by a factor of 1,000, and the results are compared against the original results of Garrels and McKenzie (1967 [DIRS 123636]). Table 4.4-1 provides the initial spring water composition used in this validation test. Figure 4 from the study by Garrels and McKenzie (1967 [DIRS 123636]) has been reproduced as Figure 7.3-1 for comparison against the EBS model results.

Table 4.4-1. Composition of Sierra Nevada Spring Water Used in Validation Tests for the EBS Seepage Evaporation Model

Parameter	ppm	mol/L $\times 10^4$
SiO ₂	24.6	4.1
Ca	10.4	2.6
Mg	1.7	0.71
Na	5.95	2.59
K	1.57	0.4
HCO ₃	54.6	8.95
SO ₄	2.38	0.25
Cl	1.06	0.16
pH	6.8	
Ionic strength	0.0013 mol/L	

Source: Garrels and McKenzie 1967 [DIRS 123636], Table VI.

NOTE: At 25°C and $p\text{CO}_2 = 10^{-3.5}$ bar.

4.4.3 Deliquescence Point Comparison

To validate the equilibrium deliquescence point calculations, comparisons of the values predicted by EQ6 calculations using *Data0.ypf* Pitzer database are made with Greenspan (1977 [DIRS 104945]) and Pabalan et al. (2002 [DIRS 163067]) experimental data. The published values are shown in Table 4.4-2; in Section 7.4, those from Greenspan (1977 [DIRS 104945]) are recalculated to the same single temperature as presented by Pabalan et al. (2002 [DIRS 163067]).

Table 4.4-3. Water Identifications used in the Binning Analysis (Continued)

Abbreviated Water Name	Starting Water Composition Sample Identification	Source
sd9-2	SD-9/1184.0-1184.2/UC	GS020808312272.004 [DIRS 166569]
sd9-3	SD-9/1184.7-1184.8/UC	GS030408312272.002 [DIRS 165226]
sd9-4	SD-9/1184.8-1185.0/UC	GS020808312272.004 [DIRS 166569]
sd9-5	SD-9/1236.4-1236.8/UC	GS020808312272.004 [DIRS 166569]
sd9-6	SD-9/1275.6-1276.0/UC	GS020808312272.004 [DIRS 166569]
sd9-7	SD-9/1330.4-1330.7/UC	GS020808312272.004 [DIRS 166569]
esfperm2	ESF-HD-PERM-2/30.1-30.5	MO0005PORWATER.000 [DIRS 150930]
esfperm3	ESF-HD-PERM-3/34.8-35.1	MO0005PORWATER.000 [DIRS 150930]
permavg	ESF-HD-PERM-AVG ^a	BSC 2004 [DIRS 172463], Table 6.2-1

^a Average of porewater analyses ESF-HD-PERM-2/30.1-30.5 and ESF-HD-PERM-3/34.8-35.1.

5. ASSUMPTIONS

This section addresses the assumptions built into the engineered barrier system physical and chemical environment model and those passed into it from upstream documentation that may have significant impact on the results of this model.

5.1 DISCUSSION OF ASSUMPTIONS IN UPSTREAM DOCUMENTATION

The assumptions listed in the two primary modeling reports that feed this model were reviewed and evaluated for their potential consequences. The two reports are:

- *Drift-Scale THC Seepage Model* (BSC 2004 [DIRS 172463], Section 5)
- *In-Drift Precipitates/Salts Model* (BSC 2004 [DIRS 169863], Section 5).

Those assumptions having a potentially significant impact are addressed below.

5.1.1 Standard State of Liquid Phase (Assumption 5.1 of the IDPS Model)

Assumption: Liquid phase is at standard state.

Basis: As discussed in *In-Drift Precipitates/Salts Model* (BSC 2004 [DIRS 169863], Section 5.1), an aqueous solution at standard state has an equilibrium relative humidity equivalent to the activity of water in the aqueous solution. Standard state in this sense implies that the water-air interface is flat (i.e., that the boundary between water and air is a plane) and that the behavior of the water molecule (H_2O) is not influenced by solid surfaces in contact with the water. Adsorption and air-water interface curvature, such as the curvature of menisci caused by capillary forces, create nonstandard-state conditions with respect to vapor pressure and equilibrium relative humidity near the air-water interface (Walton 1994 [DIRS 127454]; Koorevaar et al. 1983 [DIRS 125329], pp. 67 to 68).

For the in-drift precipitates/salts (IDPS) model, nonstandard-state aqueous solutions are not considered. Only dissolved salts and temperature are considered to affect liquid-vapor equilibrium. The small amounts of water held in double layers and adsorbed to solid surfaces have negligible roles in radionuclide transport and waste package corrosion due to their near immobility. Water held by the surface tension effects of capillarity is more mobile than water in double layers or adsorbed to solids; however, even capillary forces under very dry conditions (in the range of negative 500 meters water pressure head) have a limited effect on H_2O activity in solution (Walton 1994 [DIRS 127454], pp. 3,480 to 3,481).

Confirmation Status: No further confirmation is required. Because of this limited effect, uncertainties due to the assumption that the liquid phase in the IDPS model is at standard state are negligible compared to the more-sizable uncertainties in the IDPS model and model inputs.

Use in the Model: This assumption is used throughout.

5.1.2 Equilibrium Conditions (Assumption 5.2 of the IDPS Model)

Assumption: The system is in a state of local metastable equilibrium. All aqueous and gas constituents in the model achieve and maintain local equilibrium, and most mineral phases achieve and maintain local equilibrium upon saturation. Several slow-forming and unlikely

minerals identified in *In-Drift Precipitates/Salts Model* (BSC 2004 [DIRS 169863], Section 5.2) will not precipitate upon saturation or supersaturation. The model can be used, however, to make steady-state nonequilibrium predictions with respect to relative humidity, provided the appropriate inputs are used.

Basis: Most chemical reactions included in the model occur rapidly compared to the modeling timeframe. Redox reactions, which generally are not rapid, are not included in the model. Similarly, certain mineral precipitation reactions are not expected to be rapid enough to occur to a considerable degree for the anticipated applications of the model. Mineral precipitation reactions that fall into this category are suppressed, as explained in the IDPS report (BSC 2004 [DIRS 169863], Section 6.6.2.6.4), permitting the formation of metastable mineral phases in the model.

Highly soluble nitrate and chloride salts, which are direct inputs into TSPA-LA, rapidly deliquesce, dissolve, and precipitate, and are well approximated by equilibrium modeling. As seepage changes rather slowly with time, its most recent compositions will rapidly dominate and overcome any preexisting mineral formation influence. For this reason, kinetic properties of various mineral phases need not be explicitly included in the model during drying and rewetting cycles.

Confirmation Status: No further confirmation is required because mineral precipitation reactions that fall into this category are suppressed, as explained in the IDPS report (BSC 2004 [DIRS 169863]), permitting the formation of metastable mineral phases in the model.

Use in the Model: This assumption is used throughout.

5.1.3 Repository Location (Assumption from THC model)

Assumption: The THC model results, calculated for a repository in the Tptpll lithologic unit, are applicable to all lithologies intersected by the repository drifts.

Basis: There are three bases for this assumption:

- Model simulations in an earlier version of the THC model, as alternate conceptual models (BSC 2004 [DIRS 172463], Section 6.3), modeled drifts located within the Tptpmn and Tptpll lithologic units and show that the lithology had little effect on predicted water chemistries. Although the Tptpmn simulations are not repeated with the current THC model, which uses different input parameters and differs in some ways from the earlier model, these simulations provide confidence that the current model results are applicable over the stratigraphic section intersected by the repository.
- The repository horizon within the Topopah Spring Tuff (including the Tptpll, Tptpul, Tptpmn, and Tptpln units) is relatively uniform in composition. Peterman and Cloke (2002 [DIRS 162576]) analyzed twenty core samples, in duplicate, from the cross drift within the four lithologic units constituting the repository level. All samples were compositionally similar with respect to major oxides and trace elements (Peterman and Cloke 2002 [DIRS 162576], Table 4), and normative mineral compositions (Peterman and Cloke 2002 [DIRS 162576], Table 5, Figure 4, p. 692).

Samples vary by only 2 percent in SiO_2 concentration, and plot as a tight cluster in the rhyolite field on the chemical rock classification diagram for igneous rocks (SiO_2 plotted against $\text{Na}_2\text{O} + \text{K}_2\text{O}$) (Peterman and Cloke 2002 [DIRS 162576], Figure 3, Table 4, p. 687). The tight clustering also indicates that the effect of localized mineral heterogeneity on large-scale rock compositions, due to the presence of minerals which precipitated from the vapor phase during cooling of the tuff, and low-temperature minerals, such as calcite and amorphous SiO_2 (opal), is insignificant (Peterman and Cloke 2002 [DIRS 162576], pp. 695 to 696).

- The five starting waters used in the THC seepage model simulations were chosen to represent the entire range of available porewater compositions, and include porewaters from three of the four repository-level lithologic units (Tptpmn, Tptpll, and Tptpul) (BSC 2004 [DIRS 172463], Section 6.2.2.1).

Confirmation Status: No further confirmation is required because the variability in chemistries that are provided in the other lithologies are of the same order of magnitude or less than the variability in chemistry provided by the range of porewater compositions. This assumption allows the TSPA-License Application model to implement the lookup tables derived in Section 6.9.3.

Use in the Model: This assumption is used throughout.

5.1.4 Representative Distribution of Seepage Water Compositions (Assumption from THC model)

Assumption: THC model runs using the five starting waters adequately represent all possible seepage waters.

Basis: The five starting waters were chosen from available measured porewater compositions for repository-level lithologic units. These waters cover the spread of measured compositions (BSC 2004 [DIRS 172463], Figure 6.2-4). However, porewater samples are not available from all possible locations in the repository, and available data can only be assumed to be representative of all water chemistries actually present in the repository units. This assumption is supported in part by the chemical similarity of the four TSw lithostratigraphic units that will host the repository, as described in the previous assumption. Reaction with these rocks should homogenize many reactive mineral species and make large variations in the concentrations of nonconservative aqueous species (i.e., those that are unreactive and nonvolatile) from any single unit unlikely. This assumption is borne out by the available data (BSC 2004 [DIRS 172463], Figure 6.2-4); when the five starting waters were originally chosen, only about half the data were available (BSC 2004 [DIRS 172463], Figure 6.2-4). Porewater samples collected more recently fall within the range of the previous data and cluster in a similar fashion.

Confirmation Status: No further confirmation is required because the range of input waters is representative of the waters in the host rock.

Use in the Model: This assumption is used throughout but is explicitly referenced in Section 6.13.4.

6.2.2.4 Deliquescence

Deliquescent minerals in drift dust (or evaporated salts from seepage) are of consequence because of their potential ability to change the microscale liquid environment around dust as they absorb water vapor from the air (Figure 6.2-2). The presence of liquid water and mineral saturation in solution are required for the relative humidity (expressed as a unit fraction) of the drift's atmosphere to equal the activity of water for the solution. Campbell and Smith (1951 [DIRS 163817], p. 237) state, "It is clear that if the pressure of the aqueous vapor in the atmosphere is greater than that of the saturated solution of a salt, that salt will, on being placed in the air, form a solution: it will deliquesce." Where deliquescing minerals (salts) are present in the dust, the minerals will dissolve to form a small drop or puddle of liquid water. As shown in Figure 6.2-2, the evaporative process is the reverse of deliquescence.

Figure 6.2-2. Schematic Illustration of Deliquescence and Evaporation

6.2.2.5 Determining the Range of Temperature for the Seepage Evaporation Abstraction

Drift-Scale THC Seepage Model (BSC 2004 [DIRS 172463], Figures 6.5-4, 6.5-6, and 6.5-7) shows thermal seepage constraints that indicate there can be no seepage at drift temperatures above about 100°C due to the presence of a vaporization barrier (i.e., the liquid saturation levels fall sharply towards zero). In addition to this limitation, the results of the Drift Scale Test (DST) corroborate the absence of macroscale liquid water available in the host rock at temperatures much above about 100°C (Figure 6.2-4). Figure 6.2-4 shows the observed relationship of in situ

the FEP is excluded from further consideration, or a description of the TSPA disposition if it is included. The rationale for exclusion may be based upon regulatory requirements, low probability of occurrence, or low consequence in terms of impact on calculated dose.

Coupled processes are incorporated into the P&CE model implicitly through inputs from the THC-coupled seepage model. This report describes the chemical processes at various locations in the drift that are influenced by processes (including coupled processes) in the host rock (BSC 2004 [DIRS 172463]; BSC 2004 [DIRS 169565]); an abstraction methodology that produces a chemical environment dependent upon drip shield and waste package surface temperature and humidity; and reaction with gas-phase CO₂ and precipitation, and possible deliquescence, of soluble salts. Explicit consideration was given to the chemical interactions of potential crown seepage and ground support materials (Section 6.8).

Onsager Coupled Processes—Coupled processes involving diffusion and diffusion-like processes (e.g., heat conduction) can be described in terms of the Onsager processes, which are represented by a matrix of first-order relationships (Table 6.3-1). These are fundamental processes that can occur even if the associated physical or chemical properties of the medium are temporally or spatially invariant. Onsager couplings are driven indirectly by gradients of thermodynamic state variables (e.g., temperature, pressure, chemical potential, and electrical potential) that affect chemical transport in aqueous solution. Direct transport processes are driven by the same thermodynamic-state variables in well-known relations such as Fourier's Law, Darcy's Law, Fick's Laws, and Ohm's Law. Diffusive processes dominate in Onsager-coupled processes.

Direct processes lie along the main diagonal of the table, and indirect coupled processes are off-diagonal. The existence of indirect processes is generally known from controlled experiments. Phenomenological coefficients relating gradients and fluxes for indirect coupled processes are not generally known for geologic media. Nevertheless, the indirect coupled processes shown in Table 6.3-1 are not significant to performance of the repository because the magnitudes of the associated potential gradients or fluxes in the host rock are too small. The direct processes including Darcy flow and Fickian diffusion overwhelm the indirect processes. These direct processes are included in the models used for TSPA-LA. Some of the indirect Onsager-coupled processes listed in Table 6.3-1, such as chemical osmosis (observed in clays or zeolites) or the sedimentation current in response to heating the host rock (static potentials in the host rock) have been observed at Yucca Mountain. However, the effects of these processes are relatively small, and not important to various aspects of repository performance, including the environment in which metal barriers might corrode and the possible migration of radionuclides from breached packages.

The possible effect of coupled processes (relevant to the Onsager process) on radionuclide migration has been discussed and evaluated (BSC 2004 [DIRS 169898], Section 6.2.60). The conclusion was reached that the off-diagonal processes are unimportant. The on-diagonal processes are either accounted for in current modeling for TSPA, or are excluded. That discussion is applicable to the effect of such processes acting on the chemical environment to which metal barriers are exposed. For example, no significant pressure gradients (sufficient to support significant off-diagonal type fluxes as included in Table 6.3-1) are expected between the drift wall and the waste package outer barrier, either radially or along the length of the drift (BSC

2004 [DIRS 172463], treatment of pressure). Similarly, electrical potentials affecting the chemical environment are minimal and insufficient to drive associated off-diagonal fluxes. Temperature- and chemical-potential gradients are principal drivers for the in-drift chemical environment. Existing models incorporate the relevant effects, which are more often dominated by vapor-liquid equilibrium than condensed-phase transport effects. Osmotic equilibrium in particular is dominated by vapor-liquid equilibrium, as represented by deliquescence of salts. The same effect is controlling when a drop of seepage water falls from the drift wall onto a metal barrier surface (drip shield or waste package outer barrier). The drop re-equilibrates to new conditions of temperature (higher) and relative humidity (lower). Salt separation effects may occur on a metal barrier surface owing to several factors, including temperature and RH gradients on that surface and even in the absence of such gradients due the flow of aqueous solution down a sloping surface while precipitated solids remain behind at the point of precipitation. However, vapor-liquid equilibrium at any point along such gradients or flow paths is a strong determinant of what results at any such point.

Lastly, it is worth pointing out that the Onsager framework of addressing coupled processes is nothing more than that, a framework. Other equivalent approaches can be taken that include the relevant effects. Consider for example, diffusion of solutes in aqueous solution in the case in which the system of interest includes a temperature gradient. Instead of referring to the "Soret" effect, a treatment that explicitly expresses the diffusion coefficients as temperature-dependent quantities could be used. Furthermore, Table 6.3-1 could be expanded to include the effects of analogous potential gradients, such as gravitational potential gradient.

Table 6.3-1. Onsager Couplings and Direct Transport Process Fluxes Driven by Temperature, Pressure, Chemical Potential, and Electrical Potential Gradients

Flux	Gradient			
	Temperature	Pressure	Chemical Potential	Electrical Potential
Heat Flux	Fourier's Law—heat flow in a temperature gradient	Thermal filtration—heat flow in a pressure gradient	Dufour effect—heat flow in a density gradient	Peltier effect—heat flow in a voltage gradient
Volume Flux	Thermal Osmosis—volume flow in a temperature gradient	Darcy's Law—volume flow in a pressure gradient	Chemical Osmosis—volume flow in a concentration gradient	Electro-osmosis—volume flow in a voltage gradient
Mass Flux	Soret effect—particle flow in a temperature gradient	Reverse Osmosis—mass flow in a pressure gradient	Fick's Law—Mass flow in a concentration gradient	Electrophoresis—mass flow in a voltage gradient
Electrical Flux	Seebeck effect—electrical current in a temperature gradient	Streaming current—electrical current in a pressure gradient	Sedimentation Current—electrical current in a density gradient	Ohm's Law—Current flow in a voltage gradient

Source: Carnahan 1987 [DIRS 138706], p. 2.

NOTE: Onsager couplings and direct transport processes are along the diagonal in bold type. The Onsager couplings are important only when aqueous, liquid, or solid diffusion dominates over advection.

6.4 INTRODUCED MATERIALS

Figure 6.4-1 shows the general configuration of materials introduced into a repository drift. As seen, the current emplacement drift configuration contains no cementitious materials. The

Table 6.5-3. Minerals Allowed to Precipitate in the Engineered Barrier System Physical and Chemical Environment Geochemical Modeling (Continued)

Mineral	Formula	Criteria Selected	Rationale	References
Stellerite	$\text{Ca}_2\text{Al}_4\text{Si}_{14}\text{O}_{36} \bullet 14\text{H}_2\text{O}$	Criterion 3	Stellerite is a zeolite mineral commonly associated with fracture linings at Yucca Mountain.	Carlos et al. 1995 [DIRS 105213]
Phillipsite	$\text{K}_{0.7}\text{Na}_{0.7}\text{Ca}_{1.1}\text{Al}_{3.6}\text{Si}_{12.4}\text{O}_{32} \bullet 12.6\text{H}_2\text{O}$	Criterion 3	Phillipsite is a zeolite mineral commonly associated with evaporite deposits.	Hay et al. 1966 [DIRS 105965]
Kieserite	$\text{MgSO}_4 \bullet \text{H}_2\text{O}$	Criterion 3	Kieserite is an evaporite mineral commonly found in salt deposits. Often it is associated with halite or carnallite.	Palache et al. 1951 [DIRS 162280], pp. 477 to 479

6.6 INCOMING SEEPAGE COMPOSITION ABSTRACTION

The required seepage water and gas compositions inputs for in-drift chemistry modeling were abstracted from THC model outputs of time-dependent seepage water compositions and gas-phase compositions in the host rock (near field environment) adjacent to the drift wall. A discussion of the model used to derive these compositions is presented in *Drift-Scale THC Seepage Model* (BSC 2004 [DIRS 172463]), hereafter referred to as the THC seepage model. The THC seepage model is based on a specific design basis thermal load and thermal decay rate, which are a function of repository loading and ventilation (BSC 2004 [DIRS 172463], Section 4.1.7.3).

A time-history of seepage water compositions is calculated with the THC model for each of five compositions of porewater in the host rock, located far enough away from the drifts, at any given time interval, for liquid water presence. Because of the number of water samples collected is too small to associate a probability of occurrence (BSC 2004 [DIRS 172463], Figure 6.2-4 for a Piper plot of all available samples), the five samples are given equal probability. Those five porewater compositions are designated as (BSC 2004 [DIRS 172463], Section 6.2.2.1):

- w0 = HD-Perm water (Alcove 5)
- w4 = Cross-drift water CS2000/16.5
- w5 = Cross-drift water CS1000/7.3
- w6 = Borehole water SD-9/990.4
- w7 = Cross-drift water CS500/12.0.

The results of this model are abstracted further from where *Post-Processing Analysis for THC Seepage* (BSC 2004 [DIRS 169858]) left off, as described in this section to capture the time- and temperature-dependent changes in drift boundary conditions.

6.6.1 Conceptual Framework Summary for the Thermal-Hydrological-Chemical Seepage Abstraction

The composition of water potentially seeping into the drift is a primary influence on the type of brine produced after evaporation. For example, if the alkalinity of the water is more than twice the calcium concentration (molar basis), the water will tend to evaporatively evolve into a

Source DTN: LB0302DSCPTHCS.002.

Figure 6.7-1. In-Drift Crown Air Fraction from THC Seepage Model for All Five Starting Waters

6.7.1.2 Mass Balance: Flux Versus Corrosion Consumption

A mass balance, based on one-meter length of drift, is calculated to determine the potential for the development of oxygen deficient conditions in the drift. The calculation involves (1) an estimate of oxygen flux into the drift through the walls and along the axis of the drift, and (2) estimates of oxygen consumption due to corrosion of the emplaced materials at corrosion rates specified in Section 6.4. Oxygen consumption due to microbial activity is expected to be low compared to oxygen consumption due to corrosion. Similarly to the discussion in *Evaluation of Potential Impacts of Microbial Activities on Drift Chemistry* (BSC 2004 [DIRS 169991], Section 6.5.1 and Equation 6-4) with impact upon CO₂ generation as compared to flux, O₂ consumption (the same reaction generating CO₂) will be much less than the oxygen flux.

The estimate of oxygen flux begins with calculating the gas flux across the drift wall and into the drift, based on results from *Drift-Scale THC Seepage Model* (BSC 2004 [DIRS 172463]). The THC model presents values of flux into (or out of) the drift at the crown, side, and base of the drift at each time step (DTN: SN0407T0510102.017, *gas flux.xls*, Tab "fractures-th," Columns Titled "Gflux"). The total flux is estimated by applying the greatest inward flux to one-quarter of the drift wall and assuming outward flux through the opposite quarter, and zero flux along the two adjacent quarters. The THC model does not take into account flow along the axis of the drift and, therefore, taking the net flow into the drift, which would be an underestimation of the actual flux that might be expected in a three-dimensional drift. Additionally for waste package corrosion, convective and diffusive flux of oxygen along the axis of the drift would be expected because waste package breaches will develop at different times; therefore, areas with corrosion occurring is surrounded by oxygen-rich environments in which corrosion is not occurring.

The oxygen flux is calculated using the following values (DTN: LB0302DSCPTHCS.002 [DIRS 161976], *thc6_w0_drift_r.xls*):

- Gas flux at the crown, base, and side of the drift
- Mass fraction of air in the gas (with the remainder being water vapor)
- Volume fraction of CO₂ in the gas
- The surface area of the drift wall for which the gas-flux calculation was performed.

The following inputs are also needed (as listed in Tables 4.1-16 and 4.1-17):

- The volume fraction of oxygen, nitrogen, and argon in the earth's atmosphere (Weast and Astle 1979 [DIRS 102865], p. F-211)
- The atomic weights of the elements (Parrington et al. 1996 [DIRS 103896], pp. 62 to 63)
- The diameter of an emplacement drift (BSC 2004 [DIRS 169058])
- Size specifications of emplacement drift invert steel materials (Table 4.1-10)
- 21-PWR waste package length and separation distances
- Surface area and density of 21-PWR low-alloy steel components.

The resulting gas flux rates are plotted in Figure 6.7-2, which shows the molar O₂ and CO₂ gas fluxes into the drift per year per linear meter of drift (DTN: SN0407T0510102.017, *gas flux.xls*). The flux drop at 50 years is due to the thermally generated water vapor displacing air outward from the drifts. At 2,000 years, the gas flux increases, which also causes the O₂ and CO₂ to increase. This increase coincides with the temperature dropping significantly below 100°C (approximately 91°C) and, with the return of the liquid saturation in the rock, to values similar to pre-emplacement levels (Figures 6.5-3, 6.5-6, and 6.5-7; BSC 2004 [DIRS 172463]).

In order to perform a steady-state estimate of the oxygen partial pressure an average flux rate must be imposed. Examination of Figure 6.7-2, with the emphasis being from 50 through perhaps 200 or 300 years, resulted in the reasonable selection of a value of 3 mol/yr·m of drift for the oxygen flux.

The order of the corrosion reaction of oxygen on bare and passive iron is very nearly unity. This means that the corrosion activity effectively decreases in direct proportion to the partial pressure of oxygen. The conceptual basis for this calculation is from a corrosion study that explicitly investigated its dependence upon oxygen pressure (Jovancicevic and Bockris 1986 [DIRS 168509], Figure 6). This dependence is very linear and deviation from this at sub-atmospheric levels shows lower corrosion activity occurring. Therefore, a strict linear dependence will result in a cautious overestimation of oxygen consumption and predict a lower oxygen fugacity than might actually be expected. This is a reasonable approach as the results are for screening out the potential for anoxic conditions to occur within the drift.

6.11 ALTERNATE CONCEPTUAL MODELS

Within the P&CE model several submodels are discussed and developed; these models are the seepage evaporation abstraction, dust deliquescence abstraction, and gas abstraction. Three alternate conceptual models were investigated, two for seepage and one for dust, as discussed in the following subsections. No alternate conceptual model for the gas abstraction model is presented in this document and is screened out for the following reason:

- **In-Drift Gas**—The in-drift gas abstraction is consistent with the chemistry of the incoming seepage compositions as provided by *Drift-Scale THC Seepage Model* (BSC 2004 [DIRS 172463]). For a discussion of alternate models of THC processes, see Section 6.3 of the THC seepage model. Analyses have shown that the repository is likely to remain an oxygen-rich environment throughout the repository lifetime (Section 6.7).

6.11.1 Alternate Binning of Seepage

This alternative model discusses the abstraction of THC seepage waters based on clustering the waters by their identity and amount of precipitated carbonates, chlorides, nitrates, and sulfates present upon evaporation to dryness, rather than binning by aqueous elemental concentrations. Results of the alternative conceptual model are summarized in Section 6.11.2. The effectiveness of each approach was evaluated using the standard deviation as a percent of the mean (the coefficient of variation) for each bin. The mean value of the coefficient of variation is lower for the aqueous binning case for the pH and for the five solutes Ca, F, N, S, and Si, and is lower for the mineral clustering for the six solutes Al, C, Cl, K, Mg, and Na.

However, pH, Ca, N, and Cl are of primary importance when evaluating and determining corrosive properties and corrosion rates for the TSPA-LA. Aqueous binning gives a lower uncertainty (mean coefficient of variation) for all of these except Cl. Furthermore, the mean coefficient of variation for Cl in aqueous binning is only 0.24 percent higher than for mineral clustering (Table 6.11-7). Additionally, F and S can be inhibitors or enhancers of corrosion and it is desirable to have the least amount of uncertainty for these species, as with pH, Ca, N, and Cl. Aqueous binning gives less uncertainty (mean coefficient of variation) for both F and S. Based on these findings it was decided to use aqueous binning in the P&CE model.

In this alternate THC seepage model abstraction methodology, the output mineralogy extracted from the EQ6 calculation runs (Table 6.6-1) is used, instead of binning based on aqueous chemistry as discussed in Sections 6.6.4 and 6.6.5. The “normalized” mineral assemblages are used to classify or define a group of resulting output waters. The approach presented below relies entirely on the statistical analysis of the “normalized” output without considering any other geochemical parameters. If successful, the statistically based method will analytically determine the best binning criteria to use for defining the bins. However, the intrabin variances produced using this alternate method are generally larger than those reported in Section 6.6, so this alternate binning model will not be used.

In the analysis outlined in the following subsection, two terms are frequently used: bins and clusters. A bin is defined as a group of THC model output waters with similar physical or chemical characteristics (Section 6.6.4), which appear to be from related geochemical groups, as

6.12 EVALUATION OF KEY UNCERTAINTIES

There are four primary inputs to the EBS P&CE model, and each has uncertainty associated with it. These inputs are the:

- Composition of seepage water entering the drift. A set of potential seepage waters is abstracted from the suite of possible water compositions determined by *Drift-Scale THC Seepage Model* (BSC 2004 [DIRS 172463]), and uncertainty in the water compositions is propagated into the P&CE model. Additional uncertainty is associated with the binning process used within the P&CE model to further abstract the water compositions into 11 representative waters.
- Composition of dust that is predicted to settle on the drip shield and waste package, and of the brines that form by deliquescing salt minerals within the dust. As with the seepage waters, the uncertainty in this input is associated with the binning process, in which the possible brines are abstracted into six representative waters.
- *In-Drift Precipitates/Salts Model* (BSC 2004 [DIRS 169863]) and its associated databases (thermodynamic data, modeling assumptions, and other technical information not specific to the site) used in the geochemical modeling of seepage water evaporation and brine formation by dust deliquescence that produces the model output.
- Composition and flux of in-drift gases.

The atmosphere in the drift, in particular the concentration of CO₂, will affect in-drift water compositions.

These inputs are used in the P&CE model to estimate the compositions of potential in-drift waters, which in turn are used in the TSPA-LA to evaluate drip shield and waste package corrosion, radionuclide solubility, and colloid stability. The following five parameters are extracted from the P&CE model output and passed as direct input to the TSPA-LA:

- Chloride ion concentration
- Chloride to nitrate ion molar ratio
- Ionic strength
- pH
- Deliquescence relative humidity—the RH value at which salt minerals in the dust will deliquesce and an aqueous phase forms.

Of the four P&CE model inputs, three have uncertainties that must be propagated into the parameters that are passed to the TSPA-LA: the composition of seepage waters, composition of aqueous solutions that could form due to dust deliquescence, and the IDPS model. The remaining one, the composition of the in-drift atmosphere, has been screened out. Potential factors affecting composition and flux of in-drift gases, including corrosion of the committed materials, are

evaluated in Section 6.7. The effects of corrosion are transient; following a short period of oxygen depletion (100 to 400 years), the repository atmosphere becomes oxidizing and remains so thereafter. Uncertainties in CO₂ concentration are found to be implicitly propagated by the use of the THC seepage inputs as explained in Section 6.12.1. Thus, uncertainties in these inputs are propagated to TSPA-LA feeds by the random selection of the starting water and associated gas composition lookup tables.

The effects of corrosion of engineered materials on water chemistry is evaluated in Section 6.8, and found to be of low consequence. Thus, minor changes in repository design and the amounts of engineered materials have no effect on model uncertainty.

In the following sections, the ranges and distributions of the relevant uncertainties are developed, and implementation guidance is provided for propagating these uncertainties into the TSPA-LA parameter feeds.

6.12.1 Uncertainties and Variabilities in the Inputs from THC Model Calculations

The incoming seepage water and gas composition abstraction presented in Section 6.6 incorporates the range of effects due to uncertainties and variability in the THC model by including all five THC model input water compositions (w0, w4, w5, w6, and w7) in the abstraction. The choice of input water compositions covers the natural variability of pore-water compositions in the repository units, so the relative spread in predicted water compositions, and in the CO₂ partial pressures in equilibrium with them, is in most cases larger than the spread introduced by THC model and model input uncertainties. *Drift-Scale THC Seepage Model* (BSC 2004 [DIRS 172463], Sections 6.2.2.1, 6.6.2, and 8.1) offers the following insights:

6.2.2.1 Initial Porewater and Pore-Gas Chemistry, p. 6-15:

“The choice of input water composition must also consider the natural variability of pore-water compositions in the repository units. This natural variability is illustrated in Figure 6.2-4.”

“Given these considerations, several initial water compositions have been selected for use in the current THC seepage model based on the following criteria:

(1) Capture the spread of porewater compositions shown on Figure 6.2-4 and include, to the extent practicable, waters that may yield different end-brine compositions...”

6.6.2 Evaluation of Model Result Uncertainty, p. 6-128:

“In this study, the spread in predicted concentrations of aqueous species and CO₂ (i.e., Figures 6.5-11–6.5-20 and 6.5-24–6.5-37) is related to:

- The natural variability of input water compositions (Sections 6.2.2.1)

6.13.1 Engineered Barrier System Seepage Chemistry

Section 6.9 describes the development of seepage evaporation model lookup tables that represent the pH, I, and chemical compositions (Ca, Na, K, Mg, Al, F, S, Si, N, Cl, and C) of crown seepage and seepage wicking into the invert. Appendix B contains figures that show the various chemical parameters as a function of relative humidity and concentration factor as well as the results from the 99 individual evaporation lookup tables. The results from the lookup tables are summarized as follows:

- Section 6.13.1.1 describes the distribution of starting water that would define which set of bin history maps could be used at any given time
- Section 6.13.1.2 discusses what these lookup tables represent and the ranges of outputs associated with these tables.

6.13.1.1 Engineered Barrier System Seepage Chemistry Constraints

The THC seepage model output (Table 4.1-13) is calculated at a discrete location in the repository associated with the Topopah Spring tuff lower lithophysal zone (Tptpl) (BSC 2004 [DIRS 172463]). The assumption is made for this report, as discussed in Section 5.1.4, that the starting waters taken from the THC model, and therefore their subsequent abstraction, can be applied throughout the repository as representing the full range of possible seepage water chemistries.

The five starting waters selected by the THC seepage model for use in their model (the same five waters used in this P&CE model), represent the range of chemistries in the plotted data. Therefore, each of the five starting waters (w0, w4, w5, w6, and w7) is assigned a 20 percent probability of being selected as the starting water for a given realization. The selection of a starting water also dictates the bin history that a given model realization uses. The bin histories are located in Section 6.6.6 (Tables 6.6-8 through 6.6-12). Selecting a starting water also establishes what the starting $p\text{CO}_2$ lookup table is for a given model realization. These lookup tables are found in Section 6.7.2.1 (Tables 6.7-1 through 6.7-5). The bin history maps and $p\text{CO}_2$ lookup tables are produced for two source locations: crown seepage and invert wicking.

In-drift temperatures and relative humidity are calculated in *Multiscale Thermohydrologic Model* (BSC 2004 [DIRS 169565]). The model results presented here are generalized, and results are discussed in terms of ranges. Aside from the overall calculated ranges, specific ranges are discussed in Sections 6.13.4 and 6.13.5 for the five periods that are reported in Table 6.13-3. This provides the reader with compositional trends through time.

6.13.1.2 Engineered Barrier System Seepage Chemistry Response Surface Ranges

The set of seepage evaporation lookup tables developed and described in Section 6.9 are combined into one large lookup table to assess the overall ranges of model outputs. This combined lookup table, documented in DTN: MO0304SPACPSLT.000, defines 11 multidimensional response surfaces, one for each of the representative bin seepage waters. From these response surfaces, IDPS model outputs can be interpolated for water

are described in Section 6.12.3. Uncertainty specific to the interpolation of lookup tables, as is done for both the seepage and dust abstractions in TSPA, is evaluated in Section 7.2.2 and found to be small, and much less than the model uncertainty from the IDPS model.

Documentation of the dust deliquescence abstraction includes defensible assumptions (Section 5) and simplifications in model development (addressed in Sections 6.2, 6.5, and 6.12). The Dust Deliquescence Abstraction maintains consistency with physical principles, such as conservation of mass and energy, through the use of EQ3/6 software (Section 6.5.1).

7.1.1.3 Gas Abstraction

Development of the model is documented in accordance with the requirements of Section 5.3.2(b) of AP-SIII.10Q. Confidence building includes the following:

1. *Selection of input parameters and/or input data, and a discussion of how the selection process builds confidence in the model.* [AP-SIII.10Q, 5.3.2.(b)(1)]

Discussion of the input parameters for the gas abstraction and the bases for their selection are covered in Section 4.1. The key gas-phase species that affects the in-drift chemical environment is CO_2 . Other constituents of the gas phase are either inert for abiotic reactions in the environment (e.g., nitrogen gas, noble gases), or they are involved in reactions that do not significantly affect the bulk chemical environment (e.g., oxygen), or they are too scarce. As documented in Section 6.7.2 the CO_2 partial pressures for the in-drift chemical environment are taken from the THC seepage model, which explicitly represents the coupled chemical processes in the host rock. The amounts of moisture and CO_2 in the host rock far exceed the amounts in the drift air and the invert, and there is a continuous exchange flux between them, so it is appropriate to select the THC seepage model CO_2 pressure as the best representation of in-drift $p\text{CO}_2$.

2. *Description of initial and boundary conditions runs, and/or run convergences, and a discussion of how the activity or activities build confidence in the model. If appropriate, include a discussion of impacts of any non-convergence runs.* [AP-SIII.10Q, 5.3.2.(b)(2)]

The gas abstraction obtains $p\text{CO}_2$ directly from the THC seepage model, which is separately validated (BSC 2004 [DIRS 172463], Section 7). No additional model calculations potentially involving initial or boundary conditions, or nonconvergences, are used.

3. *Discussion of the impacts of uncertainties to the model results.* [AP-SIII.10Q, 5.3.2.(b)(3)]

The gas abstraction sets the in-drift oxygen fugacity equal to atmospheric (21% of the total pressure) as a convenient means of representing oxidizing conditions in the drift, for purposes of simulating the evolution of seepage, imbibed waters in the invert, and dust deliquescence. For this to be representative the oxygen fugacity must be shown to be great enough that key redox reactions are not significant. The IDPS model defines this

independently on bicarbonate in the EQ3 runs, thereby setting the bicarbonate concentration regardless of the input value entered.

One of the 40 waters was deemed inappropriate for modeling due to a lack of data. Specifically, in sample *ecrb6* (Table 4.4-3) the value for nitrate was given as exactly 0.0, whereas any other of the analyses supplied a detection limit (e.g., < 0.2 mg/L). As an absolute zero value for nitrate is unreasonable, and either the detection limit should be indicated or the measurement was not performed, this water is excluded from this analysis.

The binning analysis was carried out to reconfirm that the chemistries of the five starting waters used in the THC model are a good representation of the 39 water chemistries from stratigraphic units at repository depths (includes the rock units Tptpul, Tptpmn, Tptpll, and Tptpln only). The five starting waters for the THC model are designated as w0, w4, w5, w6 and w7 in Section 6.6. The 39 starting waters used in binning the repository horizon porewaters are given in Table 4.4-3, along with the associated DTNs where the water chemistry data can be located. The five THC waters are included in this binning analysis. The “w0” THC water was created by taking the average chemistries of two other waters in this binning analysis (Table 4.4-3; BSC 2004 [DIRS 172463], Table 6.2-1).

The evaporations were performed following the same procedure used in the THC seepage water abstraction in Section 6.6.3. Specifically for these porewaters the temperature was fixed at 25°C to represent their ambient condition and charge balancing was done on bicarbonate. Carbon dioxide partial pressure was fixed at the original compositions’ equilibrium value and held constant through the evaporation. The input and output EQ3/6 files are all contained with DTN: MO0406MWDARHPW.000.

Waters are then chemically grouped into bins based on the criteria given in Section 6.6.4 and Table 6.6-3. The binning analysis results of the 38 repository-horizon porewaters shows that 33 of the 38 porewaters (86.8 percent) are distributed in either bin 5 or bin 7 after evaporation to 65 percent RH, with bin 7 being the most likely chemistry to occur (Table 7.2-1). Additionally, four of the five THC starting waters are also distributed in bins 5 and 7 (80 percent). The more deleterious water chemistry, as represented by porewater bins 2 and 3 (13.2 percent), are overrepresented by the single bin 2 THC starting water chemistry (20 percent). Also, as the single difference between bins 2 and 3 lies in the criterion comparing calcium to potassium, where bin 2 is the more deleterious with calcium greater than potassium, having a bin 2 and not 3 starting THC water can also overrepresent potential risk for localized corrosion.

This comparison adds confidence that the five THC starting waters utilized in the THC model (BSC 2004 [DIRS 172463]) are a good representation of the range in near-field chemistries that are reasonably present.

report does not address dimensionality of the abstractions as they relate to water contacting engineered barriers. This report includes consideration of potential impacts of design features such as ground support degradation on in-drift water composition (Section 6.8) and the effects of chemistry coupled with transport (Section 6.11.2). In addition, treatment of alternative conceptual approaches (Section 6.11) is consistent with engineered barrier design and other engineered features. For those design or site features not incorporated in the P&CE model, analyses were done to ensure that there were no adverse impacts caused by their exclusion (see Section 6.14, as well as the relevant FEPs report for further details).

(8) *Adequate technical bases are provided, including activities such as independent modeling, laboratory or field data, or sensitivity studies, for inclusion of any thermal-hydrologic-mechanical-chemical couplings and features, events, and processes;*

This report summarizes the implicit inclusion of coupled processes by usage of the THC model output. This includes brief evaluation of all Onsager coupled processes, which are dominated by diffusion-like processes (Section 6.3). This report also includes the sensitivity analysis of how corrosion products from ground support materials impact in-drift chemistry takes into account various thermal-hydrological-mechanical-chemical effects, as do the corrosion rates (Section 6.8). However, this report contains no information on activities involving independent modeling.

(9) *Performance-affecting processes that have been observed in thermal-hydrologic tests and experiments are included into the performance assessment. For example, the U.S. Department of Energy either demonstrates that liquid water will not reflux into the underground facility or incorporates refluxing water into the performance assessment calculation, and bounds the potential adverse effects of alteration of the hydraulic pathway that result from refluxing water;*

The effects observed in thermal-hydrologic tests and experiments (from the drift scale test) are used for validation purposes in *Drift-Scale THC Seepage Model* (BSC 2004 [DIRS 172463], Section 7.1). Results from this thermal-hydrological validated model that include refluxing are used in this report (Section 6.6) to generate results used by TSPA-LA (Sections 6.12 and 6.13).

(10) *Likely modes for container corrosion (Section 2.2.1.3.1 of the Yucca Mountain Review Plan) are identified and considered in determining the quantity and chemistry of water entering the engineered barriers and contacting waste forms. For example, the model abstractions consistently address the role of parameters, such as pH, carbonate concentration, and the effect of corrosion on the quantity and chemistry of water contacting engineered barriers and waste forms;*

As indicated in Section 1.2, one of the intended uses of this model is to provide quantified inputs for ionic strength, chloride and nitrate concentrations, and pH as functions of RH , pCO_2 , and temperature to TSPA-LA. This information is then used in conjunction with another model supplying the RH and temperature information to then implement a third model, *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (BSC 2004

[DIRS 172463], Sections 6.2.2.1, 6.6.2, and 8.1) discuss the uncertainty of model conceptualizations involving the THC abstraction. The uncertainty evaluation is consistent with available site-specific data, laboratory experiments, field studies, natural analog data and process-level modeling studies. In addition, model validation is based on available site characterization data, laboratory experiments and natural analogues (Section 7). The treatment of conceptual model uncertainty described in this report does not under represent risk.

- (4) Adequate consideration is given to effects of thermal-hydrological-mechanical-chemical coupled processes in the assessment of alternative conceptual models. These effects may include:
 - (i) Thermal-hydrologic effects on gas, water, and mineral chemistry;
 - (ii) Effects of microbial processes on the engineered barrier chemical environment and the chemical environment for radionuclide release;
 - (iii) Changes in water chemistry that may result from the release of corrosion products from the waste package and interactions between engineered materials and ground water; and
 - (iv) Changes in boundary conditions (e.g., drift shape and size) and hydrologic properties, relating to the response of the geomechanical system to thermal loading;

The effects of coupled processes were considered during the assessment of alternative conceptual models (Section 6.11). The descriptions in Section 6.11 are brief because the primary evaluation of most of these alternative models (e.g., effects of microbial processes on the in-drift chemical environment) was outside the scope of this report. References are provided to the other pertinent reports. However, Section 6.11 provides details on an investigation of an alternative method for clustering waters during the abstraction of THC seepage waters. This alternative method incorporates coupled thermal-hydrological-chemical processes.

8.4.1.5 Acceptance Criterion 5—Model Abstraction Output is Supported by Objective Comparisons

- (1) *The models implemented in this total system performance assessment abstraction provide results consistent with output from detailed process-level models and/or empirical observations (laboratory and field testings and/or natural analogs);*

Information provided to the TSPA-LA was developed using detailed process-level models (Section 6.2). The resulting abstracted model output provided for implementation in the TSPA-LA is consistent with the related process-level model output (Section 7). For appropriate cases, validation against empirical observation is also provided (Section 7).

- (2) *Abstracted models for coupled thermal-hydrological-mechanical-chemical effects on seepage and flow and the engineered barrier chemical environment, as well as on the chemical environment for radionuclide release, are based on the*

- Brasher, D.M. and Mercer, A.D. 1968. "Comparative Study of Factors Influencing the Action of Corrosion Inhibitors for Mild Steel in Neutral Solution, I. Sodium Benzoate." *British Corrosion Journal*, 3, 120-129. London, England: British Joint Corrosion Group. TIC: 236434. 100883
- Brookins, D.G. 1988. *Eh-pH Diagrams for Geochemistry*. New York, New York: Springer-Verlag. TIC: 237943. 105092
- Bruno, J.; Duro, L.; de Pablo, J.; Casas, I.; Ayora, C.; Delgado, J.; Gimeno, M.J.; Peña, J.; Linklater, C.; Pérez del Villar, L.; and Gómez, P. 1998. "Estimation of the Concentrations of Trace Metals in Natural Systems. The Application of Codissolution and Coprecipitation Approaches to El Berrocal (Spain) and Poços de Caldas (Brazil)." *Chemical Geology*, 151, 277-291. Amsterdam, The Netherlands: Elsevier. TIC: 246492. 110969
- BSC (Bechtel SAIC Company) 2003. *Repository Design Project, Repository/PA IED Emplacement Drift Committed Materials (2)*. 800-IED-WIS0-00302-000-00A. Las Vegas, Nevada: Bechtel SAIC Company. ACC: ENG.20030627.0004. 164101
- BSC 2004. *D&E / PA/C IED Emplacement Drift Configuration and Environment*. 800-IED-MGR0-00201-000-00B. Las Vegas, Nevada: Bechtel SAIC Company. ACC: ENG.20040326.0001. 168489
- BSC 2004. *D&E / PA/C IED Subsurface Facilities Committed Materials*. 800-IED-WIS0-00302-000-00B. Las Vegas, Nevada: Bechtel SAIC Company. ACC: ENG.20040318.0031. 169058
- BSC 2004. *D&E/PA/C IED Typical Waste Package Components Assembly*. 800-IED-WIS0-00202-000-00C. Las Vegas, Nevada: Bechtel SAIC Company. ACC: ENG.20040517.0008. 169472
- BSC 2004. *Dissolved Concentration Limits of Radioactive Elements*. ANL-WIS-MD-000010 REV 03. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20041109.0006. 169425
- BSC 2004. *Drift-Scale THC Seepage Model*. MDL-NBS-HS-000001 REV 03. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20041201.0008. 172463
- BSC 2004. *EBS Radionuclide Transport Abstraction*. ANL-WIS-PA-000001 REV 01. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20041118.0006. 169868
- BSC 2004. *Engineered Barrier System Features, Events, and Processes*. ANL-WIS-PA-000002, Rev. 03. Las Vegas, Nevada: Bechtel SAIC Company. 169898