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Engineered Barrier System: Physical and Chemical Environment

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Engineered Barrier System: Physical and Chemical Environment

ANL-EBS-MD-000033 REV 03

November 2004

OCRWM	MODEL SIGNATURE PAGE/CHANGE HISTORY	Page iii
		1. Total Pages: 598

2. Type of Mathematical Model

☒ Process Model

☐ Abstraction Model

☐ System Model

Describe Intended Use of Model

The principal intentions of this model and analysis activity are:

- Evaluate the changes in the chemical environment that affect drip shield degradation, waste package degradation, and radionuclide migration through the invert.
- Provide valid models that will be used for the future integration of EBS thermal, hydrological, and chemical (THC) processes, which directly support the TSPA model.
- Evaluate uncertainties associated with the model.

3. Title

Engineered Barrier System: Physical and Chemical Environment

4. DI (including Rev. No., if applicable):

ANL-EBS-MD-000033 REV 03

5. Total Appendices

Five (5)

6. No. of Pages in Each Appendix

A-8, B-58, C-52, D-50, E-8

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13. Remarks

This revision has addressed and incorporated Errata 001 from the previous REV 02.

Appendix A (Block 6) includes output DTNs as electronic media on a single CD ROM.

Acknowledgements: This current Revision 03 has had significant assistance from David Shields. The previous Revision 02 was originated by Darren Jolley and technically supported by (alphabetically): Russell Jarek, Carlos Jove-Colon, Paul Mariner, and Richard Metcalf.

Change History

14. Revision No.	15. Description of Change
00	Initial Issue.
00 ICN 01	Editorial changes in Response to AP-7.5Q acceptance review. Also corrected DTN in Section 6.1.8. Replaced DTN: GS961108312771.002 with DTN:MO0005PORWATER.000 for composition of pore water sample in Section 4.1.2.2. Editorial changes throughout.

01	Revised for no-backfill design, and to include FEPs and IRSR analyses, and to address data qualification issues in Sections 4 and 5. Thermal-hydrology calculations are taken from another AMR, and discussions were added for fungal observations from the ECRB and the prediction of minerals formed by drying waters from THC calculation. Water compositions were re-calculated using a Pitzer model.
02	Revision to address removal or replacement of non-LA product input (i.e. historical TPO or other information).
03	Revision to address Regulatory Integration Team comments to enhance transparency. The in-drift oxygen balance was re-calculated, and model validation was augmented by inclusion of additional pore water analyses. Change bars were not used because the changes were too extensive to track.

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ACRONYMS AND ABBREVIATIONS

Acronyms

ANC	acid neutralizing capacity
DIRS	Document Input Reference System
DRH	deliquescence relative humidity
DTN	data tracking number
EBS	engineered barrier system
ESF	Exploratory Studies Facility
FEPs	features, events, and processes
IDPS	in-drift precipitates/salts
IED	information exchange drawings
LA	license application
P&CE	physical and chemical environment
$p\text{CO}_2$	partial pressure of CO_2
RH	relative humidity
SAW	Simulated Acidified Water
SCW	Simulated Concentrated Water
SDW	Simulated Dilute Water
SNF	spent nuclear fuel
THC	thermal-hydrological-chemical
TSPA	total system performance assessment
TSPA-LA	total system performance assessment-license application
UZ	unsaturated zone
YMP	Yucca Mountain Project

ACRONYMS AND ABBREVIATIONS (CONTINUED)

Abbreviations

atm	atmosphere
Eh	redox potential
K	Kelvin
kg	kilograms
kg/L	kilograms per liter
kg/m	kilograms per meter
Log Q/K	saturation indices
mg/L	milligrams per liter
mg/m	milligrams per meter
mm	millimeter
pe	electron activity
pH	negative log ₁₀ of hydrogen ion activity
ppm	parts per million

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 169856]) 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).

Within this model, chemical speciation calculations use equilibrium and reaction-path modeling of evaporation into highly concentrated brines to determine potential system water compositions (Na-K-H-Mg-Ca-Al-Cl-F-NO₃-SO₄-Br-CO₃-SiO₂-CO₂-O₂-H₂O). Model conditions are variable, with temperatures from 25°C to more than 140°C, pressures in the atmospheric range, and relative humidity from 0 to 100 percent.

Seepage water and gas composition inputs for in-drift chemistry modeling are 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. An abstraction method is used to generate lookup tables for key measures of possible in-drift water compositions, incorporating the effects of seepage water evaporation and deliquescence of salt minerals in dust as functions of temperature, *RH* and *pCO*₂.

Part of this abstraction process includes sorting seepage water and dust leachate compositions into bins. Each bin contains a group of seepage water or dust leachate compositions that yield chemically similar solutions when concentrated by evaporation. A water composition in each bin is identified as a "median water," which serves to approximate all of the water compositions in the group.

In addition to the water composition tables, tables are prepared using THC model output to estimate time-dependent in-drift and invert carbon dioxide partial pressure (*pCO*₂) associated with seepage compositions. An appropriate in-drift temperature range is determined by examining time-temperature curves for four locations: the waste package surface, the drift wall surface at the crown of the drift, the base of the invert, and within the rock above the crown of the drift.

The evolution of seepage waters is affected by *RH*, *pCO*₂, and temperature. Thus, it is necessary to specify these conditions to predict equilibrium chemistries for in-drift aqueous solutions. To accomplish this, lookup tables are prepared to enable selection of predicted water chemistry as a function of seepage or leachate water chemistry (bin number), *RH*, *pCO*₂, and temperature.

In addition, the following ancillary analyses are included:

- Evaluation of the corrosion of the low-alloy or carbon steel invert materials and its effects on sequestration of oxygen to determine whether there is sufficient flux of oxygen into the drifts to maintain an oxidizing environment throughout the evolution of the engineered barrier system chemical environments
- Evaluation of the corrosion of stainless steel and its effects on the composition of crown seepage waters
- Inclusion of a model to account for the potentially deleterious effects of salt (halite) separation due to transport along waste package surfaces.

Finally, other reports that either use the output of this report (directly or through its output DTNs) or are sources to this report are listed below.

Reports using this report:

- *Environment on the Surfaces of the Drip Shield and Waste Package Outer Barrier*
- *In-Package Chemistry Abstraction*
- *Total System Performance Assessment (TSPA) Model/Analysis for the License Application*
- *Igneous Intrusion Impacts on Waste Packages and Waste Forms*
- *Dike/Drift Interactions*
- *Engineered Barrier System Features, Events, and Processes*
- *Dissolved Concentration Limits of Radioactive Elements*
- *LA-SAR-1.4, Section 2.3.5.*

Reports that are sources to this report:

- *Post-Processing Analysis for THC Seepage*
- *Engineered Barrier System Features, Events, and Processes*
- *Multiscale Thermohydrologic Model*
- *Drift-Scale THC Seepage Model*
- *In-Drift Precipitates/Salts Model*
- *Geochemistry Model Abstraction and Sensitivity Studies for the 21 PWR CSNF Waste Packages*
- *Engineered Barrier System: Physical and Chemical Environment*
- *Probability Analysis of Corrosion Rates for Waste Package Materials.*

1.3 MODEL LIMITATIONS

The ranges for the TSPA-LA lookup tables that quantify the chemical parameters of interest for seepage water or dust deliquescence are defined using three sets of $p\text{CO}_2$ (10^{-2} , 10^{-3} , and 10^{-4} bars of pressure) and multiple temperatures (40°C, 70°C, and 100°C for seepage chemistries and 40°C, 70°C, 100°C, 120°C, and 140°C for dust deliquescence), and are evaluated at approximately every two RH-percent units. The main limitations of the physical and chemical environment model involve $p\text{CO}_2$ and temperature as inputs to total system performance assessment for the license application.

When selecting chemical parameters for either seepage waters or dust deliquescence under conditions that fall within lookup tables, the parameters are estimated using linear interpolation of temperature and log-linear interpolation of $p\text{CO}_2$. Chemistry values are extrapolated for pH, ionic content, chloride, and nitrate if the $p\text{CO}_2$ exceeds the range of 1×10^{-4} to 1×10^{-2} bars established in the lookup tables. Justification for this extrapolation is provided within the $p\text{CO}_2$ limits up to 2×10^{-2} and down to 1×10^{-5} bars.

When selecting chemical parameters of seepage waters for temperatures above 100°C and below 40°C , a limited extrapolation is allowed that uses the limiting values in the 100°C or 40°C lookup tables, respectively. A comparable limitation is placed on the dust deliquescence water compositions—extrapolation below 40°C or above 140°C uses the limit values.

The lowest RH values at which chemistries are provided in the lookup tables for seepage water or dust deliquescence do not always correspond to the final eutectic point for the mixture of salt minerals present (i.e., to dryness). This is especially true when the deliquescence relative humidity falls below 40 percent, for which condition the in-drift precipitates/salts (IDPS) model is not validated (BSC 2004 [DIRS 169863], Section 7.5). (The IDPS model is valid with respect to predicted chemical conditions for RH less than 40%, but not for predicting deliquescence RH values less than 40%.) It is inherently caused by the extreme ionic strengths being modeled and the lack of some ion interaction (Pitzer) database parameters.

2. QUALITY ASSURANCE

Development of this report and supporting analyses is determined to be subject to the Office of Civilian Radioactive Waste Management quality assurance program (BSC 2004 [DIRS 171156], Section 8). Approved quality assurance procedures identified in the technical work plan (BSC 2004 [DIRS 171156], Section 4) were used to conduct and document the activities described in this report. The technical work plan also identifies the methods used to control the electronic management of data (BSC 2004 [DIRS 171156], Section 8.4) during the analysis and documentation activities.

This report investigates the effect of the in-drift physical and chemical environment on the waste isolation capability of the following safety category barriers that are important to the demonstration of compliance with the postclosure performance objective prescribed in 10 CFR 63.113 [DIRS 156605]:

- Engineered barrier system: drip shield
- Engineered barrier system: waste package
- Engineered barrier system: drift invert (ballast).

This report does not directly address either engineered or natural barriers as defined in the Q-List (BSC 2004 [DIRS 168361]). However, it does provide information to modeling activities that are important to demonstrating compliance with the performance objectives in 10 CFR 63.113 [DIRS 156605].

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3. USE OF SOFTWARE

The following software was used in the preparation of this report:

3.1 EQ3/6 V8.0

EQ3/6 Version 8.0 (STN: 10813-8.0-00 [DIRS 162228]) is a software package used to perform geochemical modeling computations encompassing fluid-mineral interactions or solution-mineral-equilibria in aqueous systems, or both. This program is used in this report to model the equilibrium dissolution and precipitation of aqueous species, elemental components, and mineral precipitates present in dusts and seepage waters in the drift. The program was run on the Windows operating system (98 and 2000) on a PC platform and its limitations are described in Sections 6.5 and 6.10. The use of this software is consistent with its intended use and within its documented validation range (SNL 2003 [DIRS 162494], Section 1). Hereafter, the code will be referred to as EQ3/6, EQ3, or EQ6 depending on the specific use in the calculations described in later sections of this document.

3.2 GETEQDATA V1.0.1

GETEQDATA V1.0.1 (STN: 10809-1.0.1-00 [DIRS 161900]) is a software routine that operates as a Microsoft Excel (97 or 2000) macro to post-process data found in EQ3/6 *.3o or *.6o output files. This program is used in this AMR to extract specified data from the EQ3/6 output files to generate lookup -tables (Excel spreadsheet files). The program was run on the Windows operating system on a PC platform. This macro is limited by the EQ3/6 output data and performs a specific extraction of data as directed at run time. The use of this software is consistent with its intended use and within its documented validation range (Jarek 2002 [DIRS 169567], Section 2.1), which is to postprocess the output files from EQ3/6 versions 7.2 or 8.0. Hereafter, the code will be referred to as GETEQDATA.

3.3 EXEMPT SOFTWARE USE

The following commercial, off-the-shelf software is used in this report to perform basic calculations and statistical operations:

- Microsoft Excel 97
- Statistica 5.1.

Microsoft Excel is used throughout the document. The individual spreadsheets are called out in the section where they were used. Statistica is only used in Section 6.11.

The results obtained from the use of Microsoft Excel and Statistica 5.1 are not dependent on the software program used. The inputs, formulas, and outputs in the Microsoft Excel and Statistica files from the DTNs could be used with other similar software products to reproduce and verify the results.

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4. INPUTS

4.1 DIRECT INPUT

If not otherwise indicated, data and parameters used in this section are specifically selected for direct use in this model.

Sections 4.1.1 and 4.1.2 identify inputs required to determine the material corrosion rates, and committed materials considered for corrosion and resulting oxygen consumption. These inputs are used to estimate the oxygen pressure conditions in the drift. Section 4.1.3 describes the primary seepage water and associated gas chemistry inputs modeled using the thermodynamic databases specified in Section 4.1.4, both of which are implemented with the in-drift evaporation and salt separation submodels that are defined in Section 4.1.5. Similarly, dust deliquescence is abstracted from the inputs identified in Section 4.1.6, and it too uses the thermodynamic databases (Section 4.1.4) and evaporation process (Section 4.1.5). The final two sections describe the inputs used for sensitivity analyses of the effects of stainless steel on seepage water (Section 4.1.7) and the trace component, bromide (Section 4.1.8).

4.1.1 Material Corrosion Rates

Committed materials deemed to have no significant impact to oxygen consumption are not included as direct input to these analyses. For example, the low corrosion and degradation activity of titanium and Alloy 22, and the small quantity of copper and aluminum are examples of why these materials will not significantly affect the demand for oxygen. Corrosion rates for low-alloy or carbon steels are direct input required for the oxygen demand calculations (Section 6.7). The inclusion of Stainless Steel Type 316L is for the direct use in the analysis of crown seepage water interactions (Section 6.8) along with inputs from Section 4.1.7.

The sources for these data, and a brief description, are provided in Tables 4.1-1 and 4.1-2 for the atmospheric corrosion of Stainless Steel Type 316L and steam corrosion of carbon or low alloy steels, respectively. The mean aqueous corrosion rates for Stainless Steel Type 316L in salt water are taken from DTN: MO0409SPAACRWP.000 ([DIRS 172059], in *aqueous-316L.xls*, tab "saltwater") as 1.939 $\mu\text{m}/\text{yr}$.

Tables 4.1-1 and 4.1-2 list the sources used in the analysis of corrosion rates in this report. Southwell and Bultman's report (1982 [DIRS 100928]) is considered "established fact" as it is a professional society monograph (*The Corrosion Monograph Series*). Qualification and justification of the use of the specific corrosion values in DTN: LL980704605924.035 [DIRS 147298], Table 4.1-2 and additionally documented in McCright (1998 [DIRS 114637] Section 2.2.6, Supplements 1 and 2), is given in Appendix E of this report and was carried out as described in the data qualification plan included as a facsimile in Section E.7.

Table 4.1-1. Description of Conditions and Sources for Stainless Steel Type 316L Corrosion Rate Data Used

Temperature (°C) ⁷	Relative Humidity (RH) ⁷	Exposure Time (years)	Note	Measured Rate (various units)	Source
approx 27	approx 83%	1	1	<0.3 um loss	Southwell and Bultman 1982 [DIRS 100928] ⁸
approx 27	approx 83%	2	1	<0.3 um loss	Southwell and Bultman 1982 [DIRS 100928] ⁸
approx 27	approx 83%	4	1	<0.3 um loss	Southwell and Bultman 1982 [DIRS 100928] ⁸
approx 27	approx 83%	8	1	<0.3 um loss	Southwell and Bultman 1982 [DIRS 100928] ⁸
approx 27	approx 83%	16	1	<0.3 um loss	Southwell and Bultman 1982 [DIRS 100928] ⁸
approx 27	approx 83%	1	2	0 g/m ²	Southwell et al. 1976 [DIRS 100927], Table 5
approx 27	approx 83%	2	2	0 g/m ²	Alexander et al. 1961 [DIRS 162265], Table 2
approx 27	approx 83%	4	2	0 g/m ²	Alexander et al. 1961 [DIRS 162265], Table 2
approx 27	approx 83%	8	2	0 g/m ²	Southwell et al. 1976 [DIRS 100927], Table 5
approx 27	approx 83%	16	2	0 g/m ²	Southwell et al. 1976 [DIRS 100927], Table 5
approx 27	approx 83%	1	3	1 g/m ²	Southwell et al. 1976 [DIRS 100927], Table 7
approx 27	approx 83%	4	3	7 g/m ²	Southwell et al. 1976 [DIRS 100927], Table 7
approx 27	approx 83%	16	3	54 g/m ²	Southwell et al. 1976 [DIRS 100927], Table 7
approx 27	approx 83%	1	3	1 g/m ²	Southwell et al. 1976 [DIRS 100927], Table 7
approx 27	approx 83%	4	3	4 g/m ²	Southwell et al. 1976 [DIRS 100927], Table 7
approx 27	approx 83%	16	3	66 g/m ²	Southwell et al. 1976 [DIRS 100927], Table 7
approx 27	approx 83%	1	2	0 g/m ²	Southwell et al. 1976 [DIRS 100927], Table 7
approx 27	approx 83%	4	2	0 g/m ²	Southwell et al. 1976 [DIRS 100927], Table 7
approx 27	approx 83%	16	2	35 g/m ²	Southwell et al. 1976 [DIRS 100927], Table 7
approx 27	approx 83%	1	2	0 g/m ²	Southwell et al. 1976 [DIRS 100927], Table 7
approx 27	approx 83%	4	2	0 g/m ²	Southwell et al. 1976 [DIRS 100927], Table 7
approx 27	approx 83%	16	2	50 g/m ²	Southwell et al. 1976 [DIRS 100927], Table 7
15.78	—	5	4	0.0013 mils/yr	Bomberger et al. 1954 [DIRS 163699], Table II
15.31	—	5	5	0 mils/yr	Bomberger et al. 1954 [DIRS 163699], Table II
12.5	—	4.92	6	0.0003 mils/yr	Bomberger et al. 1954 [DIRS 163699], Table II

NOTES: ¹Panama Canal Zone, coastal exposure.

²Panama Canal Zone, inland exposure.

³Panama Canal Zone, coastal exposure (Stainless Steel Type 316/316 couple).

⁴Kure Beach, NC, shore rack 80 ft from breakers.

⁵Kure Beach, NC, main lot 800 ft from breakers.

⁶Bridgeport, Connecticut.

⁷Temperature (approx 27°C) and RH (approx 83%) approximated by taking the average value of January through December from Southwell and Bultman 1982 [DIRS 100928], Figure 64.1. The actual values of temperature and RH corresponding to each month are not given on Figure 64.1, but rather were estimated from the temperature and RH values at the beginning of each month on the graph, and then averaging these values.

⁸Southwell and Bultman 1982 [DIRS 100928], Table 64.6.

Table 4.1-2. Description of Conditions and Sources for Low-Alloy or Carbon Steels Corrosion Rate Data Used

Temperature (°C)	Relative Humidity (RH)	Exposure Time (yr)	Note	Rate (microns/year)
90	near 100%	0.5	1	241.82
90	near 100%	0.5	1	321.82
90	near 100%	0.5	1	257.97
90	near 100%	0.5	1	238.11
90	near 100%	0.5	1	195.23
90	near 100%	0.5	1	192.02
90	near 100%	0.5	1	185.47
90	near 100%	0.5	1	228.28
90	near 100%	0.5	1	228.04
90	near 100%	0.5	1	276.51
90	near 100%	0.5	1	175.85
90	near 100%	0.5	1	269.12
90	near 100%	1	1	342.99
90	near 100%	1	1	363.36
90	near 100%	1	1	358.68
90	near 100%	1	1	423.06
90	near 100%	1	1	190.72
90	near 100%	1	1	139.58
90	near 100%	1	1	133.91
90	near 100%	1	1	121.31
90	near 100%	1	1	144.45
90	near 100%	1	1	132
90	near 100%	1	1	146.48
90	near 100%	0.53	2	150.33
90	near 100%	0.53	2	210.6
90	near 100%	0.53	2	313.05
90	near 100%	0.53	2	166.22
90	near 100%	0.53	2	261.61
90	near 100%	0.53	2	203.28
90	near 100%	0.53	2	75.29
90	near 100%	0.53	2	93.33
90	near 100%	0.53	2	102.31
90	near 100%	0.53	2	129.12
90	near 100%	0.53	2	180.84
90	near 100%	0.53	2	218.57
90	near 100%	1.01	2	212.81
90	near 100%	1.01	2	193.28
90	near 100%	1.01	2	272.06
90	near 100%	1.01	2	80.15
90	near 100%	1.01	2	120.81
90	near 100%	1.01	2	168.75

Table 4.1-2. Description of Conditions and Sources for Low-Alloy or Carbon Steels Corrosion Rate Data Used (Continued)

Temperature (°C)	Relative Humidity (RH)	Exposure Time (yr)	Note	Rate (microns/year)
90	near 100%	1.01	2	72.96
90	near 100%	1.01	2	85.05
90	near 100%	1.01	2	87.64
90	near 100%	1.01	2	113.86
90	near 100%	1.01	2	146.72
90	near 100%	1.01	2	220.08

Source: DTN: LL980704605924.035 [DIRS 147298], qualified in Appendix E.

NOTES: ¹ Simulated Concentrated Well Water.

² Simulated Concentrated Well (SCW) J-13 well water.

See *atmospheric.xls* (Output DTN: MO0407SPAPCEML.005) for more details of input usage.

Representative low-alloy or carbon steel is considered similar to ASTM A 516/A516M-01 2001 [DIRS 162723], Table 1.

The other sources of direct input for corrosion rates are justified below per the requirements of AP-SIII.10Q and are considered to be qualified for the intended use in this document. The main criteria used for data qualification are corroborating data and technical assessment. Within the scope of the latter criterion, added confidence in the data is given by its publication in peer reviewed journals and its development in nationally recognized scientific institutions. Descriptions of suitability for intended use for each source are given below:

Alexander, A.L.; Southwell, C.R.; and Forgeson, B.W. 1961 [DIRS 162265]. "Corrosion of Metals in Tropical Environments."

This paper was published in the journal, *Corrosion*, a peer-reviewed journal of the National Association of Corrosion Engineers, and was presented at the 17th annual conference of the National Association of Corrosion Engineers in 1961. The Naval Research Laboratory also published it as *NRL Report 5517*. The authors from the Naval Research Laboratory performed these experiments using established engineering practices as described in the article. Tests were carried out on materials of specific interest in waste package corrosion (in particular Stainless Steel Type 316) in drift-relevant waters types of interest (dilute and salt/concentrated waters). Two values of Stainless Steel Type 316 corrosion loss, both 0.0 (zero) g/m² were taken from Table 2 of this paper, and added to the "316" worksheet in DTN: MO0407SPAPCEML.005. These values contribute to the selected mean value. They represent no sample weight loss over 2- and 4-year durations. The data for Stainless Steel Type 316L in humid air and atmospheric corrosion rates are consistent with and corroborated by the data from the other sources listed in Table 4.1-1 (output DTN: MO0407SPAPCEML.005, values within "316" worksheet).

Bomberger, H.B.; Cambourelis, P.J.; and Hutchinson, G.E. 1954 [DIRS 163699]. "Corrosion Properties of Titanium in Marine Environments."

This article was published in *Journal of the Electrochemical Society*, a peer-reviewed journal of a professional society whose area of expertise includes the corrosion of metals. The three Stainless Steel Type 316 values taken from Table II in this publication are each the average of three specimens. The values have been added to the "316" worksheet of *atmospheric.xls* of output DTN: MO0407SPAPCEML.005. The test durations were five years, and four years eleven months. Preparation methods and test conditions are described. The experiments were performed on various materials of specific interest in waste package corrosion in waters of interest (salt/concentrated waters) and atmospheric conditions. The data for Stainless Steel Type 316L humid air and atmospheric corrosion rates are consistent with and corroborated by the data from the other sources listed in Table 4.1-1 and the "316" worksheet of output DTN: MO0407SPAPCEML.005.

Southwell, C.R.; Bultman, J.D.; and Alexander, A.L. 1976 [DIRS 100927]. "Corrosion of Metals in Tropical Environments - Final Report of 16-Year Exposures."

This article describes the results of 16-year tests of a wide variety of materials, including copper and Stainless Steel Type 316, in tropical seawater (total and intermittent submersion). The article was published in *Materials Performance*, an official publication of the Corrosion Society, the National Association of Corrosion Engineers.

Authors from the Naval Research Laboratory performed the tests using established engineering practices. Tests were carried out on materials of specific interest in waste package corrosion (copper and Stainless Steel Type 316) in waters types of interest (dilute and salt/concentrated waters). Coastal and inland corrosion values from Tables 5 and 7 were added to the "316" worksheet of the output DTN. The Stainless Steel Type 316 corrosion values are corroborated and consistent with the other sources listed in the Stainless Steel Type 316L section of Table 4.1-1 and values listed in the output DTN.

4.1.2 Committed Low-Alloy or Carbon Steel Materials

Section 6.7.1 estimates to what extent the partial pressure of oxygen might change because of the fast corrosion of low-alloy or carbon steels. This involves a quantitative description of the low-alloy or carbon steel materials that are emplaced within the drift and within a representative waste package (output DTN: SN0407T0510102.017).

The only significant source of low-alloy or carbon steel within the emplacement drift—excluding the waste package and internal components—is found within the invert structure. These structural elements and their size specifications are listed in Table 4.1-10. Size specifications are used to calculate the surface areas of each component to determine its oxygen demand from corrosion. This is described in Section 6.7 and calculated in this report (output DTN: SN0407T0510102.017). Some of the minor (in terms of mass) structural components were not included as a simplification, because of nonspecific size specifications and because they account for less than 10 percent of the total material. The mass included in Table 4.1-10

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 169856]). 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 169856], 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	thc6_w0_r.xls	HD-PERM water (Alcove 5)
W4	thc6_w4_r.xls	Cross-drift water CS2000/16.5
W5	thc6_w5_r.xls	Cross-drift water CS1000/7.3
W6	thc6_w6_r.xls	Borehole water SD-9/990.4
W7	thc6_w7_r.xls	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
thc6_w0_r.xls thc6_w0_drift_r.xls	HD-PERM water (Alcove 5)
thc6_w4_r.xls thc6_w4_drift_r.xls	Cross-drift water CS2000/16.5
thc6_w5_r.xls thc6_w5_drift_r.xls	Cross-drift water CS1000/7.3
thc6_w6_r.xls thc6_w6_drift_r.xls	Borehole water SD-9/990.4
thc6_w7_r.xls thc6_w7_drift_r.xls	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 169856]), as listed in Table 4.1-15. The complete set of results in the dataset includes gas flux at the base,

side, and the crown (DTN: LB0302DSCPTHCS.002 [DIRS 161976], *thc6_w0_drift_r.xls*). To measure the flux of gas coming into the drift, the largest positive flux value, regardless of its position in the drift (side, base, or crown), is used at each time step in the calculations (output DTN: SN0407T0510102.017, *gas flux.xls*). Table 4.1-15 summarizes the position in the drift where the maximum flux occurred, CO₂ volume fraction, gas flux, and air mass fraction.

Table 4.1-15. Time-Varying Inputs for the Gas Flux Calculation in Section 6.7.1

Time (Postclosure-Years)	Position in Drift (at the Wall)	CO _{2(g)} Volume Fraction	Gas Flux (kg/s)	Air Mass Fraction
0.0027	Base	9.29E-04	-5.09E-09	9.80E-01
1	Side	1.33E-03	2.15E-09	9.40E-01
5	Side	1.26E-03	4.56E-09	9.03E-01
10	Side	1.20E-03	4.83E-09	8.92E-01
20	Side	1.09E-03	3.89E-09	8.94E-01
30	Side	9.98E-04	2.88E-09	9.02E-01
40	Side	9.97E-04	2.08E-09	9.10E-01
50	Side	9.75E-04	1.50E-09	9.17E-01
51	Side	5.01E-04	1.05E-07	2.75E-01
53	Crown	2.10E-04	1.12E-07	9.19E-03
55	Side	1.17E-04	2.71E-08	2.75E-03
60	Crown	2.58E-05	9.51E-08	3.49E-05
75	Crown	9.33E-05	3.70E-08	1.56E-03
100	Crown	2.59E-04	2.03E-08	1.81E-02
150	Crown	5.19E-04	2.94E-08	5.18E-02
200	Crown	5.99E-04	5.10E-08	6.71E-02
250	Crown	4.92E-04	3.52E-08	7.04E-02
300	Crown	3.60E-04	2.22E-08	6.49E-02
350	Crown	2.95E-04	1.59E-08	5.99E-02
400	Crown	2.95E-04	1.31E-08	5.37E-02
500	Crown	4.46E-04	1.12E-08	4.31E-02
600	Crown	8.09E-04	1.07E-08	3.96E-02
650	Crown	1.13E-03	1.38E-08	3.30E-02
700	Crown	1.48E-03	1.42E-08	3.46E-02
751	Crown	1.87E-03	1.36E-08	4.02E-02
790	Crown	2.10E-03	1.34E-08	4.57E-02
801	Crown	2.30E-03	1.33E-08	4.75E-02
1,001	Crown	4.13E-03	1.20E-08	9.23E-02
1,201	Crown	5.24E-03	1.14E-08	1.29E-01
1,401	Crown	6.37E-03	9.90E-09	1.83E-01
1,601	Crown	7.19E-03	8.47E-09	2.42E-01
1,801	Crown	7.74E-03	7.37E-09	2.86E-01
2,001	Side	7.71E-03	4.37E-08	2.17E-01
2,202	Base	7.94E-03	3.29E-08	3.01E-01
2,402 ^a	Base	8.34E-03	3.34E-08	3.57E-01
3,002	Base	7.94E-03	2.80E-08	4.84E-01
5,003	Base	6.81E-03	2.13E-08	7.01E-01
7,005	Base	7.02E-03	1.87E-08	8.00E-01
10,007	Base	7.15E-03	1.67E-08	8.73E-01

Table 4.1-15. Time-Varying Inputs for the Gas Flux Calculation in Section 6.7.1 (Continued)

Time (Postclosure Years)	Position in Drift (at the Wall)	CO _{2(g)} Volume Fraction	Gas Flux (kg/s)	Air Mass Fraction
12,310	Base	6.69E-03	1.59E-08	9.01E-01
15,010	Base	5.92E-03	1.51E-08	9.23E-01
20,013	Base	4.59E-03	1.42E-08	9.46E-01
27,355	Base	3.42E-03	1.34E-08	9.61E-01
30,020	Base	3.02E-03	1.32E-08	9.64E-01
50,035	Base	2.24E-03	1.24E-08	9.74E-01
77,206	Base	1.92E-03	1.19E-08	9.79E-01
100,067	Base	1.68E-03	1.17E-08	9.80E-01

Source: DTN: LB0302DSCPTHCS.002 [DIRS 161976], *thc6_w0_drift_r.xls*, tabs "fractures-ch" and "fractures-th."

NOTE: Negative gas flux means flux is away from the drift.

^a For time of 2402 yr (Base) two values for CO_{2(g)} volume fraction exist within the source DTN: LB0302DSCPTHCS.002 [DIRS 161976], *thc6_w0_drift_r.xls*, tab "fracture-ch." The higher value 8.34E-3 was chosen over the lower value 8.15E-3.

Oxygen Demand—The effects of corrosion of engineered barrier system (EBS) committed materials on the concentration of oxygen in the drift atmosphere through time are evaluated in two ways. One utilizes the THC seepage model output DTN: LB0302DSCPTHCS.002 [DIRS 161976] and its air fraction to calculate the lowest oxygen partial pressure resulting from displacement by thermally generated steam. The second combines the material inputs from Section 4.1.2 with the additional information in Tables 4.1-16 and 4.1-17. For these gas abstraction methodologies, see Section 6.7.1 and calculation results in output DTN: SN0407T0510102.017.

Table 4.1-16. Constant Inputs for Calculations from Section 6.7.1

Parameter	Value	Location in DTN	Source
Atomic Weight of O	15.9994 g/mol	<i>gas flux.xls</i>	Parrington, et al. 1996 [DIRS 103896], pp. 62 to 63
Atomic Weight of C	12.0107 g/mol		
Atomic Weight of N	14.00674 g/mol		
Atomic Weight of H	1.00794 g/mol		
Atomic Weight of Ar	39.948 g/mol		
Atomic Weight of Fe	55.845 g/mol	<i>Oxygen Demand.xls</i>	
Volume fraction of O ₂ in atmospheric air	0.20946	<i>gas flux.xls</i>	Weast and Astle 1979 [DIRS 102865], p. F-211
Volume fraction of N ₂ in atmospheric air	0.78084		
Volume fraction of Ar in atmospheric air	0.00934		
Cross-sectional area at wall (crown and side)	0.3605 m ²	<i>gas flux.xls</i>	LB0302DSCPTHCS.002 [DIRS 161976], <i>thc6_w0_drift_r.xls</i> tab "notes"
Cross-sectional area at wall (base)	0.5417 m ²		
Drift diameter	5.5 m	<i>gas flux.xls</i>	BSC 2004 [DIRS 169058], Figure 1

Table 4.1-16. Constant Inputs for Calculations from Section 6.7.1 (Continued)

Parameter	Value	Location in DTN	Source
21-PWR waste package length	5.0244 m	<i>Oxygen Demand.xls</i>	BSC 2004 [DIRS 169472], Table 1
Spacing between waste packages	0.1 m	<i>Oxygen Demand.xls</i>	BSC 2004 [DIRS 168489], Table 1
Density of carbon or low-alloy steels	7.85 g/cm ³	<i>Oxygen Demand.xls</i>	ASTM G 1-90 1999 [DIRS 103515], Table X1.1
Composition of carbon or low-alloy steel (Carbon Steel Type A 516 Grade 55)	C 0.22 max; Mn 0.6 to 1.20; P 0.035 max; S 0.035 max; Si 0.13 to 0.45; Fe remainder	<i>Oxygen Demand.xls</i>	ASTM A 516/A 516M-01 2001 [DIRS 162723], Table 1

Table 4.1-17. Inputs for Calculation of Oxygen Consumption by Within-Package Corrosion Processes

21-PWR CSNF Waste Package		
Material	Surface Area (cm ²)	Location in DTN
Carbon Steel Type A516 Fuel Basket Tube	1.78E+06	<i>CSNF WP Model Abstraction.xls</i>
Carbon Steel Type A516 Guides	6.14E+05	

Source: DTN: MO0210MWDEXC01.008 [DIRS 163531].

NOTE: All data listed here are used in Section 6.7.1 and output DTN: SN0407T0510102.017, *Oxygen Demand.xls*.

4.1.4 Thermodynamic Databases

The following two datasets have been developed by YMP for geochemical modeling calculations using EQ3/6:

- *Data0.ypm.R2*: This database is found in DTN: MO0302SPATHDYN.000 [DIRS 161756]
- *Data0.yppf*: This database is found in DTN: SN0302T0510102.002 [DIRS 162572]. Its development is documented in *In-Drift Precipitates/Salts Model* (BSC 2004 [DIRS 169863], Attachment I). This dataset is used for EQ3/6 Pitzer type calculations, such as those done to calculate evaporative brine compositions and includes updated equilibrium constants (e.g., log *K*, ΔH , ΔG , and *S*) and Pitzer interaction parameters for temperatures above 25°C, and additional mineral phases, including zeolites, clays, cement phases, and minerals associated with salt deposits.

In other sections of this document, these datasets are referred to as *Data0.ypm.R2* and *Data0.yppf* data files.

4.1.5 In-Drift Evaporation

In-Drift Precipitates/Salts Model (BSC 2004 [DIRS 169863]) is documented independently of this model report. The in-drift precipitates/salts model, its assumptions (Section 5.1), and validation are a direct feed into this model. Additionally, it is the report that developed the input

DTN: MO0303SPAMEQ36.000 [DIRS 162549] listed in Table 4.1-18. Refer to *In-Drift Precipitates/Salts Model* (BSC 2004 [DIRS 169863]) for model development specifics.

The model validation range for the current in-drift precipitates/salts model is for temperatures up to 140°C, *RH* from 0 to 100 percent, and deliquescence *RH* values at 40 percent or greater (BSC 2004 [DIRS 169863], Section 1; and Section 7.5.3).

The second DTN listed in Table 4.1-18 (DTN: MO0312SPAESMUN.002 [DIRS 166329]) is developed in *In-Drift Precipitates/Salts Model* (BSC 2004 [DIRS 169863], Section 8.4) and is used as input for the geochemical model uncertainties quantified in this report (Section 6.12).

Table 4.1-18. In-Drift Precipitates/Salts Model Inputs

Source DTN	Description
MO0303SPAMEQ36.000 [DIRS 162549]	General Formats for EQ3/6 Input Files Simulating the In-Drift Precipitates/Salts Model
MO0312SPAESMUN.002 [DIRS 166329]	Estimated Model Uncertainties in the In-Drift Precipitates/Salts Model

Halite Precipitation—In order to determine the highest relative humidity at which precipitation of halite may occur, two sources are examined: DTN: LL031106231032.007 [DIRS 170605] (*ExptDRHCalcsKracekRev00c.xls*) and Greenspan 1977 [DIRS 104945], Table 2. Results are discussed in Section 6.11.2 and contained within DTN: SN0403T0503404.001.

Greenspan's (1977 [DIRS 104945]) report is from *Journal of Research of the National Bureau of Standards*, 81A. The author is a highly recognized individual in this field of work and worked for the National Bureau of Standards. The National Bureau of Standards is a federal agency that establishes the standards used in measuring the physical properties of substances; therefore, the report by Greenspan (1977 [DIRS 104945]) is considered justified for intended use here.

4.1.6 Dust Leachate Compositions

Two data sets have been used to represent dust that could be deposited on waste packages and other in-drift components. These data sets (DTNs: MO0207EBSDUSTS.020 [DIRS 162556] and MO0209EBSDUST2.030 [DIRS 162557]) contain dust leachate chemical compositions, dust particle size distributions, and quantities of accumulated dust per unit area of the exposed surface.

The data in Tables 4.1-19 and 4.1-20 were used to develop EQ3 input files used for analyses in Section 6.10.

Lower limits were placed on the *RH* for the low-temperature cases of dust leachate evaporation. These calculations were halted once down to 50 percent and 30 percent *RH* at 40°C and 70°C, respectively. These limits were determined from the many waste package temperature/relative humidity plots in *Multiscale Thermohydrologic Model* (BSC 2004 [DIRS 169565], Section 6.3.1) as these low *RH* values are not observed within the drift at low temperatures. This is also described in Section 6.10.6.2.

Table 4.1-19. Water-Soluble Cations and Anions Leached from Dust Collected Throughout the Exploratory Studies Facility (Set 1)

Lab No.	Field No.	Cl	F	NO ₃	SO ₄	Br	Ca	K	Mg	Na	Si
C-186077	SPC00573607	260	8	1,820	2,200	14	2,490	350	12.8	455	173
C-186080	SPC00573610	162	24	220	640	34	430	221	19.4	304	89.2
C-186081	SPC00573611	200	30	340	840	56	941	242	6.32	378	213
C-186082	SPC00573612	154	10	340	1,060	50	630	231	28.3	388	95.1
C-186084	SPC00573614	130	12	380	1,160	24	939	219	27.1	343	121
C-186085	SPC00573615	162	12	380	740	22	863	220	25.9	369	134
C-186086	SPC00573616	130	12	400	1,480	26	893	248	35.7	374	107
C-186087	SPC00573617	140	18	440	1,180	20	919	221	32.8	332	96.4
C-186088	SPC00573618	114	12	300	400	16	439	479	13.7	345	120
C-186089	SPC00573619	200	24	420	720	22	635	214	43.6	397	100
C-186090	SPC00573620	56	4	82	162	6	226	101	10.6	157	79.1
C-186091	SPC00573622	182	6	800	1,120	10	980	183	83.6	358	43.5
C-186092	SPC00573623	180	6	580	980	22	638	193	79.7	431	46.6
C-186093	SPC00573624	240	10	280	340	54	332	128	35.7	386	14.9
C-186094	SPC00573625	300	8	680	1340	26	974	260	79.1	617	58.7
C-186095	SPC00573626	200	14	400	660	26	575	206	34.3	415	94.9
C-186096	SPC00573627	260	32	420	1,020	34	394	237	53.4	511	65
C-186097	SPC00573628	160	8	380	620	18	480	142	34.8	287	61.2
C-186098	SPC00573629	184	10	240	360	38	268	126	26.7	346	34.5
C-186099	SPC00573630	196	8	280	480	28	392	149	42	344	27.9
C-186100	SPC00573631	220	40	260	640	64	630	150	31.4	389	82.5
C-186101	SPC00573632	220	8	114	300	28	229	101	18.9	262	42.3
C-186102	SPC00573633	114	18	62	320	22	543	80	9.76	158	97.5

Source: DTN: MO0207EBSDUSTS.020 [DIRS 162556], Table S02163_009.

Table 4.1-20. Water-Soluble Cations and Anions Leached from Dust Collected Throughout the Exploratory Studies Facility (Set 2)

Lab. No./ Sample No.	Mesh Size	ESF Local (m)	Element-Oxide (ppm)									
			Ca	Mg	K	Na	Si	Cl	Br	F	NO ₃	SO ₄
C-203112/ 00574979A	60 to 200	0	147	16.3	159	55.4	161	<24	<1.6	8	<7	<32
C-203113/ 00574979B	200 to 325		91.7	9.47	127	46.4	96.5	<24	<1.6	4	10	<32
C-203114/ 00574979C	<325		119	12.6	174	66	144	<24	<1.6	8	24	<32
C-203115/ 00574980A	60 to 200	223.7	270	34.3	193	115	169	76	<1.6	18	220	220
C-203116/ 00574980B	200 to 325		466	49.3	181	124	76.6	98	4	4	400	360
C-203117/ 00574980C	<325		1,080	80.1	206	195	176	154	8	12	640	840
C-203118/ 00574981A	60 to 200	613	772	44.1	280	188	33.4	74	4	8	116	3,800
C-203119/ 00574981B	200 to 325		1,060	39.5	389	471	287	280	44	22	360	1,000
C-203120/ 00574981C	<325		2,340	130	389	392	42.8	320	6	8	1,760	4,600
C-203121/ 00574982A	60 to 200	861	246	39.6	196	262	164	86	4	20	240	320
C-203122/ 00574982B	200 to 325		458	64.1	244	339	51.6	118	6	4	520	520
C-203123/ 00574982C	<325		1,010	99.6	345	556	99.2	170	12	6	1,000	1,060
C-203124/ 00574983A	60 to 200	1,263.2	262	23.7	281	296	94.9	114	8	12	198	380
C-203125/ 00574983B	200 to 325		770	50.8	303	425	57.3	260	10	4	540	720
C-203126/ 00574983C	<325		1,240	85.9	369	666	62.7	360	10	10	980	1,200
C-203127/ 00574984A	60 to 200	2,207.5	335	49.4	339	265	87.3	128	10	10	220	440
C-203128/ 00574984B	200 to 325		—	—	—	—	—	—	—	—	—	—
C-203129/ 00574984C	<325		—	—	—	—	—	220	18	10	500	1,040
C-203130/ 00574985A	60 to 200	5,405.4	994	65.4	303	349	248	170	20	18	340	880
C-203131/ 00574985B	200 to 325		1,260	52.4	333	461	181	168	14	22	480	1,180
C-203132/ 00574985C	<325		1,030	54.7	275	480	130	166	16	22	500	1,220
C-203133/ 00574986A	60 to 200	4,013.5	248	23.4	234	222	75.4	96	6	6	146	320
C-203134/ 00574986B	200 to 325		806	38	220	292	131	170	10	12	300	740
C-203135/ 00574986C	<325		1,190	51.4	260	408	159	220	14	18	440	1,140
C-203136/ 00574987A	60 to 200	3007	1,290	84.6	257	201	21.8	188	2	8	600	5,800
C-203137/ 00574987B	200 to 325		1,180	64.1	313	564	135	360	42	22	540	1,400
C-203138/ 00574987C	<325		1,280	70.5	288	570	143	320	32	24	520	1,480
C-203139/ 00574990A	60 to 200	6,515.2	274	19.8	186	149	44.7	88	10	8	170	500
C-203140/ 00574990B	200 to 325		434	25.9	151	186	38.9	102	16	6	220	760
C-203141/ 00574990C	<325		689	34.7	251	370	82.2	136	22	14	300	940
C-203142/ 00574991A	60 to 200	7050	281	55.4	139	128	161	88	12	22	122	440
C-203143/ 00574991B	200 to 325		319	56.8	114	121	79.4	76	10	4	156	520
C-203144/ 00574991C	<325		622	53.6	177	196	215	82	12	10	164	700
C-203145/ 00574992A	60 to 200	7,622.2	122	10.3	155	171	57.4	98	6	8	70	116
C-203146/ 00574992B	200 to 325		110	9.48	121	126	12.3	82	<1.6	2	68	124
C-203147/ 00574992C	<325		305	19.8	173	187	60.2	166	2	6	150	280

Source: DTN: MO0209EBSDUST2.030 [DIRS 162557], Table 4.

The partial pressure of CO₂ in the Earth's atmosphere is 10^{-3.5} atmospheres (approximately equal to bars) (Weast 1979 [DIRS 102865], p. F.211) used in Section 6.10.3 in performing geochemical speciation calculations for the dust leachate waters.

4.1.7 Steel Corrosion Chemistry

This section provides inputs to Section 6.8, which examines the chemical impact of the steel ground support system and its resulting corrosion products on seepage waters entering the drift. The current design calls for using Stainless Steel Type 316L sheets and rock bolts (BSC 2004 [DIRS 169058], Note 4) as the drift ground support system. The metallic elements contained within this steel are presented here along with seepage condition parameters and new chromium solid species.

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 169856], 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.

Table 4.1-23. Parameters Used to Abstract Stainless Steel Type 316L Ground Support Corrosion

Parameter	Value	Units	Source
Stainless Steel Type 316L Density	7.98	g/cm ³	ASTM G 1-90 1999, Table X1.1 [DIRS 103515]
Composition of Stainless Steel Type 316L	Fe - 65.545 ^a Cr - 16.0 to 18.0 (17 avg) Ni - 10.0 to 14.0 (12 avg) Mo - 2.00 to 3.00 (2.5 avg) Mn - 2.00, Si - 0.75 N - 0.10, P - 0.045 C - 0.03, S - 0.03	Weight Percent	ASTM A 240/A 240M-02a 2002 [DIRS 162720], Table 1
Time-dependent infiltration rates	6, 16, 25 (incrementing at 600 and 2,000 years)	mm/yr	DTN: LB0302DSCPTHCS.002 [DIRS 161976]
Fracture transition time from dry to wet drift wall conditions for the value	Approximately 2,000	yr	DTN: LB0302DSCPTHCS.002 [DIRS 161976], <i>thc6_w#_r.xls</i> , tab "distance"

^a The weight percent of Fe was calculated from Table 1 of ASTM A 240/A 240M-02a 2002 [DIRS 162720] by subtracting all alloying elements from 100. When a range is given, the average of that range is used in product output DTN: SN0312T0510102.013, *DegradationMolality.zip*, tab "Composition."

Chromium Solids—The inclusion of an amorphous chromium(III) hydroxide mineral species is required to model the effects of corrosion on incoming seepage waters; otherwise, there is no controlling solid phase available for Cr in the *Data0.ympr.R2* database (DTN: MO0302SPATHDYN.000 [DIRS 161756]). The rationale for selecting the amorphous chromium hydroxide mineral species is discussed in Section 6.8.2. In addition, the formation reaction for the mineral Eskolaite (Cr₂O₃) in the current non-Pitzer database has been recast to match that described in the source for the thermodynamic data for amorphous chromium hydroxide. The solubility parameters are listed in Table 4.1-24.

The source for these species (Ball and Nordstrom 1998 [DIRS 163015]) is a peer-reviewed journal article with rigorous screening processes, in the highly respected *Journal of Chemical and Engineering Data*, authored by well-known experts in this field. This particular article is a comprehensive review of chromium metal and its aqueous species, drawing information from many sources with as much corroboration as was available. This source is, therefore, considered justified for its intended use within this report.

Table 4.1-24. Dissolution Data for Amorphous Chromium(III) Hydroxide and Eskolaite at 25°C

Mineral	Parameter	Value	Source	Used in Output DTN
Cr(OH) ₃ (am)	Log K	9.35	Ball and Nordstrom 1998 [DIRS 163015], Table 8	SN0312T0510102.013, <i>Cr-database.txt</i>
Cr ₂ O ₃	Log K	8.52	Ball and Nordstrom 1998 [DIRS 163015], Table 8	

4.1.8 Inputs used for Sensitivity Studies

In the THC seepage model, bromide (Br^-) is a trace component that is not modeled. Because halides are of concern to corrosion modeling, it is important to know to what levels they will concentrate. As Br^- is not a modeled species, no direct output for Br^- concentration is available. Measured porewater Br^- concentrations listed in Table 4.1-25 are used in Section 6.12.4 to estimate the uncertainty that the presence of Br^- adds to the seepage water composition.

Table 4.1-25. Porewater Compositional Data Used to Evaluate the Relative Importance of Br

	Local Sample Name	SPC Number	Cl mg/L	Br mg/L
1	ECRB-SYS-CS400/3.8-4.3/UC	SPC00554610	29	<1
2	ECRB-SYS-CS400/5.6-6.2/UC	SPC00554611	21	<1
3	ECRB-SYS-CS600/3.6-4.0/UC	SPC00554612	22	<1
4	ECRB-SYS-CS1000/7.3-7.7/UC	SPC00554613	21	<1
5	ECRB-SYS-CS750/6.2-6.5/UC	SPC00554614	73	<1
6	ECRB-SYS-CS2150/5.5-6.1/UC	SPC00554615	27	<0.2
7	ECRB-SYS-CS900/5.4-5.9/UC	SPC00554616	37	<0.2
8	ECRB-SYS-CS850/5.1-5.6/UC	SPC00554617	32	<0.2
9	SD-9/990.4-991.7/UC	SPC00554618	23	<0.2
10	ECRB-SYS-CS900/3.5-4.1/UC	SPC00554619	53	0.3
11	ECRB-SYS-CS1000/12.9-14.0/UC	SPC00554620	22	<0.1
12	ECRB-SYS-CS450/5.3-6.0/UC	SPC00554621	66	0.4
13	ECRB-SYS-CS2300/4.3-4.9/UC	SPC00554622	23	<0.1
14	ECRB-SYS-CS500/12.0-16.7/UC	SPC00554800	54	0.4
15	ECRB-SYS-CS2000/16.5-21.1/UC	SPC00554801	26	<0.2
16	ECRB-SYS-CS2000/16.3-16.5/UC	SPC00554802	24	<0.2
17	ECRB-SYS-CS950/5.2-5.3/UC	SPC00554803	19	<0.2
18	ECRB-SYS-CS950/4.8-5.5/UC	SPC00554804	30	<0.2
19	SD-9/991.7-992.1/UC	SPC00554805	26	0.1
20	ECRB-SYS-CS1250/5.0-5.7/UC	SPC00554806	50	0.2
21	ECRB-SYS-CS1250/3.4-4.0/UC	SPC00554807	25	ND
22	SD-9/670.5-670.6/UC	SPC00554808	46	0.3
23	ECRB-SYS-CS800/4.9-5.6/UC	SPC00554809	20	ND
24	ECRB-SYS-CS700/5.5-5.8/UC	SPC00554810	64	<0.1
25	NRG-7/7A/839.3-839.8/UC	SPC00554811	31	0.1

Source: DTN: GS020408312272.003 [DIRS 160899].

NOTE: ND indicates "not determined."

The direct input DTN source for the data in Table 4.1-25 (DTN: GS020408312272.003 [DIRS 160899]) is also used as indirect input for validation (Table 4.4-3). This is an acceptable use of this DTN source because the validation is based upon the major aqueous ion chemistries used in the binning criteria (Section 6.6) that do not include any bromide (Br^-) in the analysis.

4.2 CRITERIA

The technical work plan (BSC 2004 [DIRS 171156]) does not state acceptance criteria relevant to this report. However, justification for models and analyses performed in this report is provided by *Project Requirements Document* (Canori and Leitner 2003 [DIRS 166275], pp. 3 to 15), which is based on 10 CFRs 63.113 and 63.114 [DIRS 156605] requirements. More-specific acceptance criteria exist in *Yucca Mountain Review Plan, Final Report* (NRC 2003 [DIRS 163274] and are presented and addressed in Section 8.4 to supplement or clarify *Project Requirements Document* (Canori and Leitner 2003 [DIRS 166275]) citations.

4.2.1 Acceptance Criteria Addressed

The following criteria are from *Yucca Mountain Review Plan, Final Report* (NRC 2003, Section 2.2.1.3.3.3 [DIRS 163274], which is based on meeting 10 CFR 63.114(a)–(c) and (e)–(g) [DIRS 156605]) requirements.

Acceptance Criterion 1–System Description and Model Integration Are Adequate

- (1) Total system performance assessment adequately incorporates important design features, physical phenomena, and couplings, and uses consistent and appropriate assumptions throughout the quantity and chemistry of water contacting engineered barriers and waste forms abstraction process;
- (2) The abstraction of the quantity and chemistry of water contacting engineered barriers and waste forms uses assumptions, technical bases, data, and models that are appropriate and consistent with other related DOE abstractions. For example, the assumptions used for the quantity and chemistry of water contacting engineered barriers and waste forms are consistent with the abstractions of “Degradation of Engineered Barriers” (Section 2.2.1.3.1); “Mechanical Disruption of Engineered Barriers” (Section 2.2.1.3.2); “Radionuclide Release Rates and Solubility Limits” (Section 2.2.1.3.4); “Climate and Infiltration” (Section 2.2.1.3.5); and “Flow Paths in the Unsaturated Zone” (Section 2.2.1.3.6). The descriptions and technical bases provide transparent and traceable support for the abstraction of quantity and chemistry of water contacting engineered barriers and waste forms;
- (3) Important design features, such as waste package design and material selection, backfill, drip shield, ground support, thermal loading strategy, and degradation processes, are adequate to determine the initial and boundary conditions for calculations of the quantity and chemistry of water contacting engineered barriers and waste forms;
- (4) Spatial and temporal abstractions appropriately address physical couplings (thermal-hydrological-mechanical-chemical). For example, DOE evaluates the potential for focusing of water flow into drifts, caused by coupled thermal-hydrological-mechanical-chemical processes;
- (5) Sufficient technical bases and justification are provided for total system performance assessment assumptions and approximations for modeling coupled thermal-

hydrological-mechanical-chemical effects on seepage and flow, the waste package chemical environment, and the chemical environment for radionuclide release. The effects of distribution of flow on the amount of water contacting the engineered barriers and waste forms are consistently addressed, in all relevant abstractions;

- (6) The expected ranges of environmental conditions within the waste package emplacement drifts, inside of breached waste packages, and contacting the waste forms and their evolution with time are identified. These ranges may be developed to include:
  - (i) Effects of the drip shield and backfill on the quantity and chemistry of water (e.g., the potential for condensate formation and dripping from the underside of the shield);
  - (ii) Conditions that promote corrosion of engineered barriers and degradation of waste forms;
  - (iii) Irregular wet and dry cycles;
  - (iv) Gamma-radiolysis; and
  - (v) Size and distribution of penetrations of engineered barriers;
- (7) The model abstraction for quantity and chemistry of water contacting engineered barriers and waste forms is consistent with the detailed information on engineered barriers design and other engineered features. For example, consistency is demonstrated for:
  - (i) Dimensionality of the abstractions;
  - (ii) Various design features and site characteristics; and
  - (iii) Alternative conceptual approaches.

Analyses are adequate to demonstrate that no deleterious effects are caused by design or site features that DOE does not take into account in this abstraction;

- (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;
- (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;

- (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;
- (12) Guidance in NUREG-1297 (Altman et al. 1988 [DIRS 103597]) and NUREG-1298 (Altman et al. 1988 [DIRS 103750]), or other acceptable approaches, is followed.

Acceptance Criterion 2—Data Are Sufficient for Model Justification

- (1) Geological, hydrological, and geochemical values used in the license application are adequately justified. Adequate description of how the data were used, interpreted, and appropriately synthesized into the parameters is provided;
- (2) Sufficient data were collected on the characteristics of the natural system and engineered materials to establish initial and boundary conditions for conceptual models of thermal-hydrological-mechanical-chemical coupled processes, that affect seepage and flow and the engineered barriers chemical environment;
- (4) Sufficient information to formulate the conceptual approach(es) for analyzing water contact with the drip shield, engineered barriers, and waste forms is provided;

Acceptance Criterion 3—Data Uncertainty Is Characterized and Propagated Through the Model Abstraction

- (1) Models use parameter values, assumed ranges, probability distributions, and bounding assumptions that are technically defensible, reasonably account for uncertainties and variabilities, and do not result in an under-representation of the risk estimate;
- (2) Parameter values, assumed ranges, probability distributions, and bounding assumptions used in the total system performance assessment calculations of quantity and chemistry of water contacting engineered barriers and waste forms are technically defensible and reasonable, based on data from the Yucca Mountain region (e.g., results from large block and drift-scale heater and niche tests), and a combination of techniques that may include laboratory experiments, field measurements, natural analog research, and process-level modeling studies;
- (3) Input values used in the total system performance assessment calculations of quantity and chemistry of water contacting engineered barriers (e.g., drip shield and waste package) are consistent with the initial and boundary conditions and the assumptions of the conceptual models and design concepts for the Yucca Mountain site. Correlations between input values are appropriately established in the DOE total system performance assessment. Parameters used to define initial conditions, boundary conditions, and computational domain in sensitivity analyses involving coupled thermal-hydrological-mechanical-chemical effects on seepage and flow, the waste package chemical environment, and the chemical environment for radionuclide

release, are consistent with available data. Reasonable or conservative ranges of parameters or functional relations are established;

- (4) Adequate representation of uncertainties in the characteristics of the natural system and engineered materials is provided in parameter development for conceptual models, process-level models, and alternative conceptual models. DOE may constrain these uncertainties using sensitivity analyses or conservative limits. For example, DOE demonstrates how parameters used to describe flow through the EBS bound the effects of backfill and excavation-induced changes;

Acceptance Criterion 4—Model Uncertainty Is Characterized and Propagated Through the Model Abstraction

- (1) Alternative modeling approaches of FEPs are considered and are consistent with available data and current scientific understanding, and the results and limitations are appropriately considered in the abstraction;
- (2) Alternative modeling approaches are considered and the selected modeling approach is consistent with available data and current scientific understanding. A description that includes a discussion of alternative modeling approaches not considered in the final analysis and the limitations and uncertainties of the chosen model is provided;
- (3) Consideration of conceptual model uncertainty is consistent with available site characterization data, laboratory experiments, field measurements, natural analog information and process-level modeling studies; and the treatment of conceptual model uncertainty does not result in an under-representation of the risk estimate;
- (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 barriers 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 engineered barriers 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

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-testing and/or natural analogs);
- (2) Abstracted models for coupled thermal-hydrological-mechanical-chemical effects on seepage and flow and the engineered barriers chemical environment, as well as on the chemical environment for radionuclide release, are based on the same assumptions and approximations demonstrated to be appropriate for process-level models or closely analogous natural or experimental systems. For example, abstractions of processes, such as thermally induced changes in hydrological properties, or estimated diversion of percolation away from the drifts, are adequately justified by comparison to results of process-level modeling, that are consistent with direct observations and field studies; and
- (3) Accepted and well-documented procedures are used to construct and test the numerical models that simulate coupled thermal-hydrological-mechanical-chemical effects on seepage and flow, engineered barriers chemical environment, and the chemical environment for radionuclide release. Analytical and numerical models are appropriately supported. Abstracted model results are compared with different mathematical models, to judge robustness of results.

4.2.2 Acceptance Criteria Not Addressed

The subcriteria from Quantity and Chemistry of Water Contacting Engineered Barriers and Waste Forms of *Yucca Mountain Review Plan, Final Report* (NRC 2003 [DIRS 163274], Section 2.2.1.3.3.3, based on meeting the requirements of 10 CFR 63.114(a)–(c) and (e)–(g) [DIRS 156605]), are not addressed within this report. The specific subcriteria, followed by reasoning for their exclusion, are presented here.

Acceptance Criterion 1—System Description and Model Integration Are Adequate

- (11) The abstraction of in-package criticality or external-to-package criticality, within the emplacement drift, provides an adequate technical basis for screening these events. If either event is included in the assessment, then the U.S. Department of Energy uses acceptable technical bases for selecting the design criteria that mitigate the potential impact of in-package criticality on repository performance; identifies the features, events, and processes that may increase the reactivity of the system inside the waste package; identifies the configuration classes and configurations that have potential for nuclear criticality; and includes changes in thermal conditions and degradation of engineered barriers in the abstraction of the quantity and chemistry of water contacting engineered barriers and waste forms;

Issues involving criticality are not addressed.

Acceptance Criterion 2—Data Are Sufficient for Model Justification

- (3) Thermo-hydrologic tests were designed and conducted with the explicit objectives of observing thermal-hydrologic processes for the temperature ranges expected for repository conditions and making measurements for mathematical models. Data are sufficient to verify that thermal-hydrologic conceptual models address important thermal-hydrologic phenomena;

This report is not used for design or conduct of thermal-hydrologic testing, and information on predicted thermal-hydrologic conditions in the repository is obtained from other reports (e.g., BSC 2004 [DIRS 169565]).

- (5) Sufficient data are provided to complete a nutrient- and energy-inventory calculation, if it has been used to justify the inclusion of the potential for microbial activity affecting the engineered barrier chemical environment and the chemical environment for radionuclide release. As necessary, data are adequate to support determination of the probability for microbially influenced corrosion and microbial effects, such as production of organic byproducts and microbially enhanced dissolution of the high-level radioactive waste glass form.

This report involves no microbial activity calculations and therefore uses no data regarding nutrient- or energy-inventory.

Acceptance Criterion 3—Data Uncertainty Is Characterized and Propagated Through the Model Abstraction

- (5) If criticality is included in the total system performance assessment, then the U.S. Department of Energy uses an appropriate range of input parameters for calculating the effective neutron multiplication factor; and

Issues involving criticality are not addressed at all within this report.

- (6) Where sufficient data do not exist, the definition of parameter values and conceptual models is based on other appropriate sources, such as expert elicitation conducted in accordance with NUREG-1563 (Kotra et al. 1996 [DIRS 100909]).

This report had no need for expert elicitation (peer review) for basis of parameter values or conceptual models. This would be performed, if required, as directed by AP-SIII.10Q, 5.3.2.(c)(4).

Acceptance Criterion 4—Model Uncertainty Is Characterized and Propagated Through the Model Abstraction

- (5) If the U.S. Department of Energy uses an equivalent continuum model for the total system performance assessment abstraction, the models produce conservative estimates of the effects of coupled thermal-hydrologic-mechanical-chemical processes on calculated compliance with the postclosure public health and environmental standards.

This report contains no specifics on TSPA-continuum modeling for coupled thermal-hydrologic-mechanical-chemical processes.

4.3 CODES, STANDARDS, AND REGULATIONS

4.3.1 Codes

This model documentation was prepared to comply with the U.S. Nuclear Regulatory Commission high-level waste rule (10 CFR Part 63 [DIRS 156605]). Subparts of this rule applicable to data include Subpart B, Section 15 (Site Characterization) and Subpart E, Section 114 (Requirements for Performance Assessment). The Subpart applicable to models is also Subpart E, Section 114. The sections applicable to FEPs are 10 CFR 63.114(d), (e), and (f).

4.3.2 Standards

The following standards are applicable to this report as they have been used as direct input in subsections of Section 4.1. The specific use of each standard is listed below with that standard's reference.

- ASTM A 240/A240M-02a 2002 [DIRS 162720], *Standard Specification for Chromium and Chromium-Nickel Stainless Steel Plate, Sheet, and Strip for Pressure Vessels and for General Applications*, was used to determine the chemical composition of the material to be used in the fabrication of the ground support (Stainless Steel Type 316L, Table 4.1-23).
- ASTM A 276-03 2003 [DIRS 165006], *Standard Specification for Stainless Steel Bars and Shapes*, was used to determine the chemical composition of the Stainless Steel Type 316L material to be used in the fabrication of the perforated sheets for the ground support.
- ASTM A 516/A516M-01 2001 [DIRS 162723], *Standard Specification for Pressure Vessel Plates, Carbon Steel, for Moderate- and Lower-Temperature Service*, was used to determine the chemical composition of the material to be used in the fabrication of the basket for the waste package.
- ASTM A 588/A588M-01 2001 [DIRS 162724], *Standard Specification for High-Strength Low-Alloy Structural Steel with 50ksi [345Mpa] Minimum Yield Point to 4-in. [100-mm] Thick*, was used to determine the chemical composition of the material to be used in the fabrication of the invert-transverse beams with stiffeners, invert-longitudinal support beams, invert-stiffener brackets, invert-base plates, invert-structural bolts, and the rail runway beams, cap plate, and guide beams for the gantry rail assembly.
- ASTM A 759-00 [DIRS 159971], *Standard Specification for Carbon Steel Crane Rails*, was used to determine the chemical composition of the material to be used in the fabrication of the gantry rail for the gantry rail assembly.

- 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 169856]), *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 169856]), 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.yypf* 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 4.4-2. Measured Deliquescence Relative Humidity Values for Salts and Salt Mixtures

Salt Composition	Temperature (°C)				
	23	38.1	48	69	85.8
^a NaNO ₃	74.9	—	69.7	62.7	—
^b MgCl ₂	33.9	31.7	31	29.1	—
^b NaCl + NaNO ₃	74.7	66.4	67.2	59.6	56
^b NaCl + NaNO ₃ + KNO ₃	67.8	60.7	61.3	51.8	43.4
Salt Composition	Temperature (°C)				
	20 to 25	35 to 40	45 to 50	65 to 70	85 to 90
^c NaNO ₃	75.36 to 74.25	72.06 to 71.00	69.99 to 69.04	66.64 to 66.04	65.03 to 65.00
^c MgCl ₂	33.07 to 32.78	32.05 to 31.60	31.10 to 30.54	28.54 to 27.77	25.11 to 24.12

Sources: ^a Pabalan et al. 2002 [DIRS 163067], Table 5-1.^b Pabalan et al. 2002 [DIRS 163067], Table 5-2.^c Greenspan 1977 [DIRS 104945], Table 2.

4.4.4 Chromium Calculation

Figure 2 from the study by Rai et al. (1987 [DIRS 163369]) has been used to validate the $\text{Cr}(\text{OH})_{3(\text{am})}$ solubility $\log K$ value obtained from Ball and Nordstrom (1998 [DIRS 163015], Table 8), and as given in Table 4.1-24 (Section 4.1.7). This figure is reconstructed here in Figure 4.4-1.

Source: Rai et al. 1987 [DIRS 163369].

NOTE: The lines represent best-fit linear regressions through 77 experimentally measured solubility data points (not shown).

Figure 4.4-1. Three-Species Model for Chromium Solubility

4.4.5 Repository Horizon Porewaters

Repository Horizon Porewaters—Starting water chemistry compositions used to model the evaporation of repository horizon porewaters are archived in five separate DTNs and one report. Table 4.4-3 provides the porewater sample identification numbers and source DTNs. The water samples that have been chosen for the analysis are those that originated from the stratigraphic rock units located at the depth of the repository horizon. These rock units include the Tptpul, Tptpmn, Tptpll, and Tptpln. In addition, the porewater samples must include pH measurements in their analyses. Other porewater samples that are archived in the listed DTNs (Table 4.4-3) are not included in the analysis, as they do not meet these criteria. These porewaters and their resulting chemical distributions are used to support validation of the selection of the five starting THC porewaters (Section 7.2.3). Throughout the remainder of this report, the waters will be referred to by their abbreviated water name (Table 4.4-3).

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

Abbreviated Water Name	Starting Water Composition Sample Identification	Source
ecrb1	ECRB-SYS-CS400/5.6-6.2/UC	GS020408312272.003 [DIRS 160899]
ecrb2	ECRB-SYS-CS450/5.3-6.0/UC	GS020408312272.003 [DIRS 160899]
ecrb3	ECRB-SYS-CS500/12.0-16.7/UC	GS020408312272.003 [DIRS 160899]
ecrb4	ECRB-SYS-CS600/3.6-4.0/UC	GS020408312272.003 [DIRS 160899]
ecrb5	ECRB-SYS-CS750/6.2-6.5/UC	GS020408312272.003 [DIRS 160899]
ecrb6	ECRB-SYS-CS800/4.9-5.6/UC	GS020408312272.003 [DIRS 160899]
ecrb7	ECRB-SYS-CS850/5.1-5.6/UC	GS020408312272.003 [DIRS 160899]
ecrb8	ECRB-SYS-CS900/3.5-4.1/UC	GS020408312272.003 [DIRS 160899]
ecrb9	ECRB-SYS-CS900/5.4-5.9/UC	GS020408312272.003 [DIRS 160899]
ecrb10	ECRB-SYS-CS950/4.8-5.5/UC	GS020408312272.003 [DIRS 160899]
ecrb11	ECRB-SYS-CS950/5.2-5.3/UC	GS020408312272.003 [DIRS 160899]
ecrb12	ECRB-SYS-CS1000/11.1-11.6/UC	GS031008312272.008 [DIRS 166570]
ecrb13	ECRB-SYS-CS1000/12.9-14.0/UC	GS020408312272.003 [DIRS 160899]
ecrb14	ECRB-SYS-CS1000/5.4-6.1/UC	GS031008312272.008 [DIRS 166570]
ecrb15	ECRB-SYS-CS1000/7.3-7.7/UC	GS020408312272.003 [DIRS 160899]
ecrb16	ECRB-SYS-CS1100/3.7-3.8/UC	GS030408312272.002 [DIRS 165226]
ecrb17	ECRB-SYS-CS1250/3.4-4.0/UC	GS020408312272.003 [DIRS 160899]
ecrb18	ECRB-SYS-CS1500/10.0-12.1/UC	GS020808312272.004 [DIRS 166569]
ecrb19	ECRB-SYS-CS2000/16.3-16.5/UC	GS020408312272.003 [DIRS 160899]
ecrb20	ECRB-SYS-CS2000/16.5-21.1/UC	GS020408312272.003 [DIRS 160899]
ecrb21	ECRB-SYS-CS-2000/3.95-4.1/UC	GS031008312272.008 [DIRS 166570]
ecrb22	ECRB-SYS-CS2150/5.5-6.1/UC	GS020408312272.003 [DIRS 160899]
ecrb23	ECRB-SYS-CS2250/5.2-5.6/UC	GS020808312272.004 [DIRS 166569]
ecrb24	ECRB-SYS-CS2300/4.3-4.9/UC	GS020408312272.003 [DIRS 160899]
ecrb25	ECRB-SYS-CS2300/6.1-6.7/UC	GS020808312272.004 [DIRS 166569]
esfsad1	ESF-SAD-GTB#1/194.2-195.2/UC	GS020808312272.004 [DIRS 166569]
esfsad2	ESF-SAD-GTB#1/195.4-196.7/UC	GS020808312272.004 [DIRS 166569]
esfther1	ESF-THERMALK-017/26.5-26.9/UC	GS031008312272.008 [DIRS 166570]
esfther2	ESF-THERMALK-017/22.9-23.0/UC	GS031008312272.008 [DIRS 166570]
nrg1	NRG-7/7A/839.3-839.8/UC	GS020408312272.003 [DIRS 160899]
sd9-1	SD-9/990.4-991.7/UC	GS020408312272.003 [DIRS 160899]

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 169856], 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 169856], 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 169856], 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 (Ttptmn, Ttptll, and Ttptul) (BSC 2004 [DIRS 169856], 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 169856], 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 169856], Figure 6.2-4); when the five starting waters were originally chosen, only about half the data were available (BSC 2004 [DIRS 169856], 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.

5.2 ASSUMPTIONS INTERNAL TO PHYSICAL AND CHEMICAL ENVIRONMENT MODEL

5.2.1 Representative Distribution of Dust and Dust Leachate Compositions

Assumption: The distribution of the aqueous leachate from 52 dust samples corresponds to a representative distribution of previously suspended dust in the Exploratory Studies Facility (ESF) drift and is representative of repository dust.

Basis: Excavation activity may generate the majority of the repository dust (Section 6.10.2), and, as this dust has a common source, it should be of similar composition to those U.S. Geological Survey samples taken from the ESF. Peterman et al. (2003 [DIRS 162819], Figure 3) indicate that the major source of the dust collected in the ESF is from the rhyolite of the Topopah Spring tuff. The dust samples themselves are similar with respect to leachate chemistries, and only six abstraction bins are needed to separate them into their major chemical groups (Section 6.10.5). In addition, processes producing soluble constituents are believed to be representative, although their relative abundance may not be. Data supporting the representativeness of the tunnel dust soluble fractions are presented in *Environment on the Surfaces of the Drip Shield and Waste Package Outer Barrier* (BSC 2004 [DIRS 161237], Table 6.7-14).

Confirmation Status: No further confirmation is required because the generally similar leachate chemistries reported in Section 6.13.4.2 indicate that the chemical variability is minor and is adequately represented by the existing data set.

Use in the Model: This assumption is used in Section 6.10.5.3.2 and 6.13.2.1.

5.2.2 Dryout Temperature for Deliquescent Dust Compositions

Assumption: The dust leachate bins 2 through 6, and their representative median waters (Table 6.10-6), are to be considered completely dry at and above the temperature of 160°C.

Basis: Dust bins 2 through 6 consist primarily of Na-K/Cl-NO₃ or a subset thereof. With the lack of reliable data directly on these multicomponent mixtures and their eutectic boiling points, this assumption is made. There are data from *International Critical Tables of Numerical Data, Physics, Chemistry and Technology* (Kracek 1928 [DIRS 105223]) that indicate the highest boiling point for the pure-salt system from the combinations possible is NaNO₃ at 120.59°C. Modeling results in *Environment on the Surfaces of the Drip Shield and Waste Package Outer Barrier* (BSC 2004 [DIRS 161237], Figures 6.7-3 and 6.7-14) indicate that the assemblage NaCl-NaNO₃-KNO₃ reasonably indicates a boiling point between 135°C to 140°C.

This assumption is needed because for certain of the dust systems, predicted dryout (deliquescence RH) is less than 40 percent, which outside the validation range of the IDPS model (BSC 2004 [DIRS 169863], Section 7.5.3).

Confirmation Status: For the NaCl-NaNO₃-KNO₃ assemblage, the best-available, current prediction of dryout conditions is at (or very close to) the validation limit of the IDPS model (140°C). Experimental data for this assemblage are needed to confirm the assumption of dryout at or below 160°C.

Use in the Model: This assumption is used to support instructions to TSPA-LA in Section 6.15.1.2.

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6. MODEL DISCUSSION

6.1 MODELING OBJECTIVES

The main purpose of the engineered barrier system (EBS) physical and chemical environment (P&CE) abstractions is to predict the evolution of the environment in the disposal drifts in response to the chemical and physical processes shaping it following repository closure. The chemical conditions can affect drip shield and waste package corrosion, radionuclide solubility, and colloidal stability. The conceptual model (Section 6.2) for the evolution of water chemistry in the EBS includes the consideration of seepage evaporation effects, interactions with engineered materials, dust deliquescence, and reactions with in-drift gases.

In general, Section 6 can be divided into three major areas of focus: 1) a set of screening analyses conducted to evaluate the effects of introduced materials on the EBS geochemical environment; 2) models developed and abstracted, with uncertainties, for use by the TSPA-LA model in evaluating engineered barrier performance and radionuclide mobility (Foldout Figure 6.1-1); and 3) additional sensitivity studies and alternate conceptual models.

One of the screening analyses provided in Section 6 consists of evaluating predominate engineered material types, compositions, and corrosion rates (Section 6.4). Section 6.4 presents corrosion rates for iron steel and alloy materials. Once the rates have been determined, most of the materials are screened out as having little potential to affect the chemical environment.

Of the introduced materials, the rock bolts and the perforated stainless steel sheets are the engineered items that could react with, and affect the chemical composition of, potential seepage before it makes contact with the drip shield or waste package outer barrier. These two items are made of stainless steel and their potential interactions with seepage water are evaluated in Section 6.8.

Also included in the screening analyses is an evaluation of the effect of the degradation of introduced materials on the in-drift gas composition (particularly O_2 ; Section 6.7). This analysis investigates whether corrosion of the introduced low-alloy or carbon steel has the potential to affect one of the main boundary conditions established for the model calculations (oxidizing conditions will be maintained in the drift).

In the remainder of Section 6, three different models are developed:

- Lookup tables to represent the partial pressure of CO_2 in the drift through time (gas abstraction, Section 6.7.2.1)
- An abstraction model to represent the chemical composition of seepage through time (seepage evaporation abstraction, Sections 6.6 and 6.9)
- A model to evaluate the deliquescence of dusts (dust deliquescence abstraction, Section 6.10).

Foldout Figure 6.1-1 diagrams the main process steps that generate the abstractions and lookup tables feeding the TSPA-LA model.

The main software tool used in the development of the seepage evaporation abstraction and the dust deliquescence abstraction is EQ3/6 Version 8.0 (STN: 10813-8.0-00 [DIRS 162228]). Section 6.5 discusses the mathematics used by the EQ3/6 calculations and some of the modeling constraints required to produce the model results used in developing the lookup tables for seepage and deliquescent dusts. The main modeling tool used in these calculations is *In-Drift Precipitates/Salts Model* (BSC 2004 [DIRS 169863]).

Sections 6.12 and 6.13 summarize the results of the modeling calculations: Section 6.12 details the uncertainties associated with key outputs as determined from *In-Drift Precipitates Salts Model* and the development of the lookup tables. Section 6.12 also documents several additional sensitivity analyses, including:

- Use of alternate mineral suppressions
- Model sensitivity to carbon dioxide partial pressure
- The presence of bromine in seepage and dusts
- Variations in the geochemical model for stainless steel-seepage interactions.

Section 6.13 summarizes and discusses the model results in terms of the potential environmental conditions on waste packages, drip shields, and in the invert. This section also discusses the potential evolution of brines, the controlling mineral phases for each brine type, and the types of water that could contact waste packages, drip shields, and the invert. Finally, there are specific instructions important to the TSPA to ensure the lookup tables can be properly implemented in the TSPA-LA model. These instructions are located primarily in Section 6.15. Three main TSPA abstraction models are outlined in this section:

- Implementation of seepage conditions on the waste package
- In the absence of seepage, the dust deliquescence model implements the dust chemistries on the waste package
- Instructions for the abstraction model in the invert are provided to use the seepage chemistry lookup tables.

Instructions for implementing uncertainty on each of these abstractions are outlined in Section 6.12.5. Some discussion on the implementation of interpolation and extrapolation between the lookup tables is discussed in Section 6.13. Alternate conceptual models and features, events, and processes (FEPs) are also discussed in Sections 6.11 and 6.14, respectively.

Major EBS-Environment Process Flowchart by Sections

Seepage Model Abstraction Process

Dust Leachate Analyses Abstraction Process

Figure 6.1-1. Major EBS Environment Process Flowchart, with Section References

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6.2 ENGINEERED BARRIER SYSTEM PHYSICAL AND CHEMICAL ENVIRONMENT CONCEPTUAL MODEL

6.2.1 Integrated Perspective on the Evolution of the Engineered Barrier System Physical and Chemical Environments

The EBS environments are important to repository performance to the extent that they help determine engineered barrier component degradation rates, quantities and species of mobilized radionuclides, and transport rates for radionuclides and fluids through the drift into the unsaturated zone (UZ). The drip shield and the waste package outer barrier are the principal performance-related engineered barrier components that initially prevent water contact with waste forms and determine fluid transport paths. The EBS chemical environment affects radionuclide solubility and colloid stability in the invert, which affect the mobile radionuclide source term for transport. Fluid transport paths and rates, coupled with the source term, determine radionuclide transport rates to the UZ.

The main purposes of this report are to provide:

- Geochemical conditions on the waste package and drip shield, where concentrated brines could potentially form through the evaporation of seepage waters and deliquescence of salt minerals in dust deposited on the metal surfaces
- Geochemical conditions in the invert, which may be used to determine the solubility and colloidal stability of radionuclides.

The evolution of the EBS environment is discussed in terms of processes (Section 6.2.2) and spatial locations (Section 6.2.3). Descriptions by process are often independent of exact spatial location in the drift. On the other hand, descriptions by spatial location may encompass multiple processes taking place within meters of each other within the drift. *In-Drift Precipitates Salts Model* (BSC 2004 [DIRS 169863]) also discusses many of these same concepts and processes.

6.2.2 Evolution of Engineered Barrier System Chemical Environment by Process

The following discussion conceptualizes potential seepage and evaporation, dust deposition and deliquescence, and the influence of temperature changes over time on the chemical environment within the drift.

6.2.2.1 Seepage

Surface waters, originating as surface precipitation and snow melt, gradually make their way downwards through fractures and the matrix of the tuffaceous rocks in the UZ to the level of the drift. During the initial radioactive decay heating pulse (extending approximately 2,000 years after the permanent closure of the repository), areas near the drift rise in temperature above 96°C, the boiling point of water for the drift elevation (Figure 6.7-7). This heating pulse drives away water as steam, resulting in some parts of the drift that do not have macroscale liquid water available for chemical reactions. This process is important because it limits aqueous corrosion on the waste package and drip shield. The process also limits the water available to transport soluble and colloidal radionuclides from the waste form.

After the maximum temperature in the drift is reached during the radioactive decay heat pulse, water can potentially flow into the drift and onto the engineered barriers from the host rock. A result of seepage during and after the heat pulse is evaporation and deposition of minerals on the surface of the waste package and drip shield. This can also cause a separation of components from the aqueous phase during transport to the invert (Section 6.11.2).

Depending on the percolation fluxes and saturation levels, the contact between the host rock and invert crushed tuff can allow water to imbibe into the invert through the permeable tuff matrix.

6.2.2.2 Chemical Divides

As seepage waters make their way into the drift, their chemical composition changes by evaporation and mineral precipitation. When minerals (including salts) precipitate, the relative concentrations of remaining dissolved components change. This effect is a result of chemical divides encountered and mineral precipitates from natural waters. Drever (1988 [DIRS 118564], p. 235) explains the chemical divide:

Whenever a binary salt is precipitated during evaporation, and the effective ratio of the two ions in the salt is different from the ratio of these ions in solution, further evaporation will result in an increase in the concentration of the ion present in greater relative concentration in solution and a decrease in the concentration of the ion present in lower relative concentration.

There are six common geochemical divides for natural lakes (Figure 6.2-1). These geochemical divides largely control the types of waters that can develop by evaporation.

Source: Drever 1988 [DIRS 118564], p.236. Note that Drever identifies dolomite or another Mg-bearing carbonate, as a possible alternative to sepiolite in this diagram.

Figure 6.2-1. Simplified Chemical Divides Diagram Based on Evaporative Concentration of Dilute Starting Waters to Form a Suite of Naturally Occurring Lake Waters

In the seepage abstraction, potential seepage waters are grouped based on the composition of the concentrated brines that form on evaporation (Section 6.6). In accordance with geochemical divide theory, the water composition changes due to the sequence of minerals that precipitate from solution. That sequence is a function of the initial water composition, the thermal conditions, and the gas composition. Evaporation to concentrated brines is simulated using geochemical speciation calculations (EQ3/6, Sections 6.5 and 6.6). These modeling results provide the suite of concentrated brine compositions that could potentially form on the waste package and drip shield.

Analogous evaporite minerals are commonly found on desert playa lakes in Nevada as the result of evaporative concentrations of relatively dilute and low-solute content rainwater and snowmelt (Papke 1976 [DIRS 162274], Table 1). For these reasons, model calculation runs simulating the evaporation of Sierra snowmelt were carried out to validate the EQ6 Pitzer brine evaporation modeling (Section 7.4). In addition, the presence of the same evaporite minerals in Nevada playas provides corroboration for the mineral assemblages predicted by the EQ3/6 software evaporative concentration computer simulations (Section 6.13.1).

6.2.2.3 Dust Deposition

During construction, ventilation, and waste package emplacement, and after sealing the primary entrances to the repository, dust will accumulate in the drift. Dust on the drip shields and waste packages is of concern for its potential influence on corrosion.

Dust is deposited initially from the tuff bedrock during excavation and construction of the repository (Section 6.10). In addition, ventilation will carry surface dust into the drifts. Surface dust contains natural evaporitic minerals, blown in from the surrounding countryside and playas, possibly from up to hundreds of kilometers away (Reheis et al. 2002 [DIRS 163132]). Some dust may contain bromide, which has been used as a tracer in construction waters at Yucca Mountain. The effect of bromide on the expected chemical environment is evaluated in Section 6.12.4.2.

Atmospheric dust has not been characterized directly as part of this project, but information in the literature on the general properties of this dust, on relevant atmospheric processes, and on materials from desert playas in Nevada, has been summarized in *Environment on the Surfaces of Drip Shield and Waste Package Outer Barrier* (BSC 2004 [DIRS 161237], Section 6.7.2.8). In general, nitrate is an important component of atmospheric dusts, primarily due to its production in the upper atmosphere by electrical phenomena. Nitrate salts are recognized as an important component of atmospheric dusts and aerosols, and their properties (including deliquescence) are considered important to the understanding of certain weather and climatic phenomena. Anthropogenic sources add to the nitrate burden of atmospheric dust. The extent to which playa dusts are incorporated within atmospheric dust is not well known. Nitrate minerals are not commonly described as components of surficial playa salts, so playas are not considered a significant source of nitrate in atmospheric dust.

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 169856], 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

moisture content with temperature, from neutron logging for the DST, in borehole 79 (February 1998 to December 2001).

Literature data and measured laboratory core sample saturations (Flint 1998 [DIRS 100033], pp. 32 to 33) are in close agreement with observations from the DST (Figure 6.2-4), and show that at 60°C and 65 percent relative humidity, rock saturation becomes low enough that liquid flow essentially stops and vapor transport predominates. In measuring volumetric water content, Flint (1998 [DIRS 100033], pp. 32 to 38) used the standard drying heat of 105°C, which is normally considered to remove most porewaters, but noted that "some, but not all, water was removed from the zeolites, clays, and pore spaces." The literature surveyed by Flint (1998 [DIRS 100033], p. 38) suggested that most of the water released from 105°C to 180°C is from thermal dehydration of zeolites, clays, and interstitial waters. These constraints indicate that the seepage evaporation abstraction is applicable for temperatures from ambient (approximately 25°C) to 100°C.

(Figure 6.2-3 intentionally deleted.)

Source: DTN: MO0406SEPTVDST.000 [DIRS 170616], 79_complete.xls.

Figure 6.2-4. Rock Moisture Content as a Function of Temperature as Measured from Neutron Logging of Borehole 79 during the DST Heating Phase

6.2.3 Conceptual Description of Engineered Barrier System Chemical Environments by Spatial Location

Figure 6.2-5 depicts several representative locations along a vertical flow path from the crown of the drift to the base of the invert where the chemical compositions of water and gas can directly affect degradation rates of the engineered barrier components, quantities and species of mobilized radionuclides, and transport rates for radionuclides and fluids through the drift into the UZ. It is at these locations that performance-related water compositions may change (to concentrated brines in some instances) due to the processes described previously.

Waste forms are contained in metal waste packages. These packages lie on pallets that rest on a flat invert composed of crushed host rock and metal beams. Titanium alloy drip shields, resting on the invert, cover the waste packages. Drip shields divert entering water, preventing it from contacting the waste packages. If a drip shield is breached, it only partially shields the waste packages from potential seepage water. Waste packages may be breached by corrosion, which may lead to degradation of the waste forms and release of radionuclides to the invert.

Several processes potentially affect the in-drift chemical environments and are relevant to performance assessment:

- Gas, water, and EBS materials interactions (Sections 6.4 through 6.10, and 6.13)
- Evaporation of water and condensation of water vapor (Sections 6.9 and 6.10)
- Salts precipitation and dissolution (Sections 6.9, 6.10, and 6.11.2).

When conditions for seepage exist, seepage water enters the drift by gravity (i.e., by dripping; Figure 6.2-5). The composition of this water is influenced by reactions with ground support materials (e.g., rock bolts, and other ground support components) and with gases in the host rock. The water then falls through the air gap above the drip shield where further reaction with in-drift gases occur. Interactions with ground support materials and reactions with gases are considered to be part of Location 1 (Figure 6.2-5).

After passing through the air gap above the drip shield, the water contacts the surface of the drip shield (Figure 6.2-5, Location 2) where it is diverted away from the waste package. On the drip shield, water evaporation, salt precipitation, transport related phase separation, and aqueous solution formation by rewetting and deliquescence of precipitated salts can occur. As long as it is intact, the drip shield will divert water fluxes around the waste packages to the invert and the UZ.

If the drip shield is breached (i.e., by uniform corrosion), seepage water can pass through the breaches and contact the surface of the waste package (Figure 6.2-5, Location 3) where it is diverted to the invert unless the waste package is breached. Potential evaporation, condensation, transport separation, and chemical processes at the surface of the waste package are the same as those for the drip shield. Aqueous solutions can initiate corrosion and corrosion products can further alter the water composition.

Water that passes through breaches in the waste package will contact the waste forms (Figure 6.2-5, Location 4). As the cladding and waste forms degrade, radionuclides will be mobilized in the water as dissolved or colloidal species. Further discussion of these issues is provided in *In-Package Chemistry Abstraction* (BSC 2004 [DIRS 167621]), *Dissolved Concentration Limits of Radioactive Elements* (BSC 2004 [DIRS 169425]), and *Waste Form and In-drift Colloids-Associated Radionuclide Concentrations: Abstraction and Summary* (BSC 2004 [DIRS 170025]).

Advection and diffusion in flowing water and condensed water films can transport radionuclide-containing species through breaches in the waste package to the invert (Figure 6.2-5, Location 5).

Water can enter the invert (Figure 6.2-5, Location 5) from:

- Direct seepage
- Diversion by the drip shield
- Diversion by the waste package
- Flow from the waste package
- Imbibition or wicking from host rock (not shown in Figure 6.2-5).

The composition of waters entering the invert (Figure 6.2-5, Location 5) determines the stable concentrations of dissolved and colloidal radionuclides, based on solubility and colloid stability models (BSC 2004 [DIRS 169425]; BSC 2004 [DIRS 170025]).

6.2.4 Engineered Barrier System Physical and Chemical Environment Conceptual Model Locations

The EBS P&CE model can be summarized by a discussion of the locations identified in the conceptual model (Figure 6.2-5). The model can be described as a series of either mixing or reaction cells that are found at the various spatial locations along the flow path, as discussed in Section 6.2.2. The various process model calculations documented or reported in Sections 6.4 through 6.10 use these reaction cells. Outputs from these sections are applied to other existing models, such as in-drift colloids and radionuclide solubility in the invert. The following subsections describe the development, application, and use of the P&CE model calculations. The actual flow and transport calculations that determine the flux and diversion within the in-drift environment can be found in *EBS Radionuclide Transport Abstraction* (BSC 2004 [DIRS 169868], Section 6.5.1.1).

6.2.4.1 Flux into Drift

The first step in developing the P&CE model is the selection of the incoming gas and water compositions for potential seepage entering through the crown of drift, as described in Section 6.6. Water compositions representing fluids wicking into the invert for the same spatial and boundary conditions are also provided for direct input into Location 5.

6.2.4.2 Location 1 (Drift Wall and Air Gap)

Potential seepage water and gas chemistries can be modified by interactions with rock bolts and steel sheets, or directly flow (drip) onto the surface of the drip shield (Location 2). In general, potential seepage water interactions with the corrosion products themselves should not significantly alter the major ion composition of the water entering the drift. To support this, sensitivity analyses of the effects of chromium released during the corrosion of Stainless Steel Type 316L have been conducted (Section 6.8).

NOTE: Not shown is the wicking of water into the invert from the host rock.

Figure 6.2-5. Schematic Illustration of Locations of Important Interfaces and Fluxes in the Engineered Barrier System

6.2.4.3 Location 2 (Surface of the Drip Shield)

A portion of the water coming from Location 1 may be diverted directly to the invert (Location 5) by the drip shield, or it may undergo evaporative processes, be influenced by any biofilms present, or react with dust and debris sitting on the drip shield. These fluids could flow onto the surface of the waste package (Location 3), but could only flow into the package (Location 4) if a pathway becomes available. The effects of evaporative processes on the potential seepage composition are modeled and discussed in Sections 6.9 and 6.13. These process model results are the primary source of chemistry for fluids contacting the waste package.

The corrosion products associated with the drip shield are not expected to adversely effect the compositions of any waters flowing off or through the drip shield due to the very slow corrosion rates for titanium and to the insoluble nature of titanium oxides (Section 6.4.2). For the same reasons, removal or addition of trace elements by sorption or dissolution processes associated with the active corrosion of the alloy is not considered.

6.2.4.4 Location 3 (Surface of the Waste Package)

Although the composition of the waste package alloy differs from that of the drip shield, it too, is highly corrosion-resistant (Section 6.4.2), and the processes occurring at Location 2 are also applicable to this location.

6.2.4.5 Location 4 (Inside Waste Package)

This portion of the conceptual process is documented in other reports such as *Summary of In-Package Chemistry Abstraction* (BSC 2004 [DIRS 167621]). The results of the model developed in that report are used as input into Location 5.

6.2.4.6 Location 5 (Invert)

The in-drift colloids model and the radionuclide solubility model require compositional parameters for water in the invert, as discussed in Section 6.13. Three incoming water sources are considered--from Locations 2 or 3 (i.e., potential seepage was modified by evaporative processes and diverted around the waste package), from Location 4, and waters wicking directly into the invert. These are provided to the TSPA-LA (Sections 6.13 and 6.15) in order to evaluate radionuclide solubility and colloid stability in the TSPA model for the invert.

6.3 COUPLED PROCESSES

Coupled processes are those in which two or more physical and chemical processes simultaneously interact to produce a result, or in which a process is affected by physical and chemical variables at the same time. The coupled processes considered in the TSPA are those that have been found to have a potentially significant effect on dose calculations.

The relative importance of different coupled processes, formally classified as FEPs, is discussed briefly in Section 6.14 and documented in more detail in various FEPs reports (BSC 2004 [DIRS 169898], Section 6.2.60). These reports contain straightforward screening arguments if

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 169856]; 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 169856], 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

materials that are emplaced are expected to undergo chemical and physical changes, and they may affect the in-drift chemical environment.

This section analyzes the corrosion rate and relative lifetime of the primary introduced materials to the current repository design. This information is used later to establish boundary conditions, modeling constraints, and potential effects upon the in-drift environment. In general, waste package and drip shield material longevity is evaluated in documentation such as *WAPDEG Analysis of Waste Package and Drip Shield Degradation* (BSC 2004 [DIRS 169996]). Evolution of the in-package materials is evaluated in *In-Package Chemistry Abstraction* (BSC 2004 [DIRS 167621]).

The chemical effects and corrosion rates of other introduced materials are evaluated within this document. The low-alloy or carbon steels are found to be the only significant contributor to the oxygen mass balance calculations associated with the evolution of the in-drift gaseous environment (Section 6.7). Alloy 22 and titanium material corrosion rates are only presented here to demonstrate their insignificant effect upon the in-drift environment. The analyses in this section also are used to determine the extent of effect on seepage chemistry as it pertains to the interaction with the ground support (e.g., Stainless Steel Type 316L corrosion in Section 6.8).

Figure 6.4-1. General Location of Engineered Barrier System Components and Materials

6.4.1 Material Corrosion Rates

In the following sections and tables, general corrosion rates under a variety of environmental conditions are discussed. These include corrosion rates determined under humid air and immersed conditions. Titanium and Alloy 22 corrosion rates are taken directly as those used by other project documents.

For other materials, a set of experimental work for the project was carried out using three waters, referred to as Simulated Dilute Water (SDW), Simulated Concentrated Water (SCW), and Simulated Acidified Water (SAW), respectively (McCright 1998 [DIRS 114637]). The SDW simulates J-13 well water at 10× concentration to account for minor effects of water evaporation and boiling. SCW simulates J-13 well water concentrated 1,000× to account for long-term water evaporation and boiling in the repository environment. SAW represents J-13 well water that has been acidified and concentrated, which is intended to simulate the effect of possible microbial metabolic products. Corrosion tests were run on samples immersed in these waters, and in the humid air generated above these waters upon heating. Further information on these simulated solutions is provided by McCright (1998 [DIRS 114637]).

The corrosion of metals in the atmosphere is primarily controlled by temperature, relative humidity, and chemistry. Many other parameters can affect corrosion rates, including time of wetness, rainfall, fog, and hours of sunlight, but these are not discussed here as such parameters are not available to describe the in-drift environment. Temperatures and relative humidity values are presented in the tables below. However, details of chemistry are not available in many cases. Note that the tables in this document capture the data as it exists within each data source as opposed to providing a consistent number of significant figures. In the case of reporting values from EQ3/6 calculated data, rounding is usually done to three significant figures.

The most corrosive environments are typically the marine and industrial atmospheres, which represent corrosion under conditions of high humidity, of metal covered with a salt crust, or in the presence of high concentrations of atmospheric contaminants.

In the case of pooled water in or on materials, those values indicated by “freshwater” and “saltwater” are used for the corrosion rate. The freshwater rates are representative of those solutions that are dilute, such as lake water and J-13 well water. The saltwater rates are for ocean water with an average chloride content of approximately 17,000 ppm (Forgeson et al. 1958 [DIRS 159343]), and are used when the natural waters have been concentrated due to evaporation or contact with engineered materials. Modifications to these definitions will be discussed for each individual material in the following sections.

6.4.1.1 Titanium

Because a stable oxide film (TiO_2) forms quickly upon exposure to oxygen, titanium is generally resistant to corrosion. This is shown in Table 6.4-2, which lists the corrosion rates of Ti (Grade 16) determined for the dripping water case in *General Corrosion and Localized Corrosion of the Drip Shield* (BSC 2004 [DIRS 169845], Table 17). These general corrosion rates of the outer surface of the drip shield are represented by a cumulative distribution function (CDF) generated by combining the Long Term Corrosion Test Facility (LTCTF) 1-year weight-loss samples and

the crevice samples from experimental results (BSC 2004 [DIRS 169845], Section 6.5.5). The minimum corrosion rate is taken as the lowest corrosion rate that is greater than zero for the CDF. The maximum corrosion rate is given as the corrosion rate that is closest to the 95th percentile for the CDF. The minimum, maximum, and 50th percentile of the CDF are shown in bold in Tables 6.4-2 and 6.4-18.

(Table 6.4-1 is intentionally deleted.)

Table 6.4-2. Titanium Grade 16 Corrosion Rates

Sample	Corrosion Rate ($\mu\text{m}/\text{yr}$)	Cumulative Distribution Function (CDF)
1	0.00E+00	0.00E+00
2	4.18E-03 (minimum)	1.43E-01
3	7.91E-03	1.79E-01
4	7.91E-03	2.14E-01
5	7.92E-03	2.50E-01
6	7.99E-03	2.86E-01
7	1.60E-02	3.21E-01
8	1.61E-02	3.57E-01
9	1.65E-02	3.93E-01
10	2.10E-02	4.29E-01
11	2.36E-02	4.64E-01
12	2.37E-02 (50 th percentile))	5.00E-01
13	2.40E-02	5.36E-01
14	2.53E-02	5.71E-01
15	4.00E-02	6.07E-01
16	4.26E-02	6.43E-01
17	4.29E-02	6.79E-01
18	5.15E-02	7.14E-01
19	6.34E-02	7.50E-01
20	6.50E-02	7.86E-01
21	7.15E-02	8.21E-01
22	7.92E-02	8.57E-01
23	8.22E-02	8.93E-01
24	1.12E-01	9.29E-01
25	1.13E-01 (maximum)	9.64E-01
26	3.19E-01	1.00E+00

Source: BSC 2004 [DIRS 169845; Table 17].

NOTE: Corrosion rates converted to $\mu\text{m}/\text{yr}$ from mm/yr .

6.4.1.2 Alloy 22

Corrosion rates for Alloy 22 given here are consistent with those determined in *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (BSC 2004 [DIRS 169984], Section 6.4.3.4), which presents a base-case temperature-dependent general corrosion model that determines general corrosion rates of Alloy 22 based on an Arrhenius

relation in logarithmic form (BSC 2004 [DIRS 169984], Equation 6-25). The calculated model output is presented as a general corrosion rate CDF at different temperatures (BSC 2004 [DIRS 169984], Figure 6-26; DTN: MO0409MWDUGCMW.000 [DIRS 171714]. Table 6.4-3 provides the 5th, 50th, and 95th percentile results of the corrosion rate CDF for Alloy 22 at 25°C, 50°C, 75°C, 100°C, 125°C, and 150°C. Table 6.4-18 provides these same results but for 25°C, 100°C, and 150°C only. The corrosion rate results in Tables 6.4-3 and 6.4-18 have been converted from nm/yr to $\mu\text{m}/\text{yr}$.

Table 6.4-3. Corrosion Rates of Alloy 22

Temperature (°C)	5 th percentile ($\mu\text{m}/\text{yr}$)	50 th percentile ($\mu\text{m}/\text{yr}$)	95 th percentile ($\mu\text{m}/\text{yr}$)
25	0.0005	0.0024	0.0058
50	0.0011	0.0053	0.0131
75	0.0021	0.0106	0.0262
100	0.0039	0.0193	0.0477
125	0.0065	0.0326	0.0805
150	0.0104	0.0518	0.1278

Source: DTN: MO0409MWDUGCMW.000 [DIRS 171714]; *Base Case GC Rate CDF.xls*, Tab: "Base Case GC Rate."

NOTE: All corrosion rates converted from nm/yr to $\mu\text{m}/\text{yr}$.

6.4.1.3 Copper Alloy

The summary of corrosion rates for copper under different environmental conditions is presented in Table 6.4-8. Under outdoor conditions, the main factors influencing corrosion of copper are relative humidity and concentration of aerosol particles (Sequeira 2000 [DIRS 162970]).

(Tables 6.4-4 through 6.4-7 are intentionally deleted.)

Table 6.4-8. Corrosion Rates of Copper Under Various Environmental Conditions

Environment	Maximum ($\mu\text{m}/\text{year}$)	Mean ($\mu\text{m}/\text{year}$)	Minimum ($\mu\text{m}/\text{year}$)
90°C, J-13 Steam, near 100% relative humidity	4.15	2.86	1.67
95°C to 100°C, J-13 Steam, near 100% relative humidity	6.60	4.79	3.15
150°C, J-13 Steam, near 100% relative humidity	1.78	1.09	0.46
90°C, Soln 7 steam, near 100% relative humidity (1,000 ppm Cl)	5.90	1.60	0.39
Marine Atmosphere (70% to 83% relative humidity)	4.14	1.68	0.43
Marine Atmosphere (60% to 70% relative humidity)	1.38	1.33	1.27
Rural Atmosphere (wet-69.5% to 83% relative humidity)	2.01	0.94	0.42
Rural Atmosphere (dry-39% relative humidity)	0.13	0.13	0.13
Industrial Atmosphere (65% to 68% relative humidity)	1.90	1.50	1.30
Urban Atmosphere (74% relative humidity)	1.40	1.22	1.04

Source: DTN: MO0312SPAPCEML.003 [DIRS 167409], *atmospheric.xls*, Tab "copper."

6.4.1.4 Aluminum Alloy

Measured aqueous corrosion rates for aluminum alloy are presented in Table 6.4-9. Aluminum differs from other metals in that the main corrosion behavior is a form of localized corrosion called pitting. Because pitting does not allow for easy determination of material lifetimes, pitting weight loss data for aluminum are converted to general rates for use in this report.

Table 6.4-9. Corrosion Rates of Aluminum Alloys in Aqueous Environments

Environment	Maximum ($\mu\text{m}/\text{year}$)	Mean ($\mu\text{m}/\text{year}$)	Minimum ($\mu\text{m}/\text{year}$)
Fresh water	36.93	12.95	0.40
Saltwater	110.91	9.69	0.12

Source: DTN: MO0409SPAACRWP.000 [DIRS 172059], *aluminum2.xls*, Tab "range."

Atmospheric data on the corrosion of aluminum alloy come from *Corrosion* (ASM International 1987 [DIRS 103753], Tables 8 and 11) and can be found in Table 6.4-10. The minimum value comes from 20-year atmospheric corrosion data, the median value from 10-year atmospheric corrosion data, and the maximum from the highest value of atmospheric corrosion.

Table 6.4-10. Atmospheric Corrosion Rates of Aluminum Alloy 6061

Maximum Rate ($\mu\text{m}/\text{year}$)	Median Rate ($\mu\text{m}/\text{year}$)	Minimum Rate ($\mu\text{m}/\text{year}$)
0.422	0.35	0.076

Source: ASM International 1987 [DIRS 103753], Tables 8 and 11.

6.4.1.5 Stainless Steel Type 316L

In relatively uncontaminated environments, such as rural atmospheres or steam produced from dilute solutions such as J-13 well water, the corrosion rate for Stainless Steel Type 316L is slow. However, when the atmosphere contains contaminants, such as chlorides, the corrosion rate rises significantly (Table 6.4-11). Chloride contamination can come from exposure to marine environments or concentrated underground waters. The amount of corrosion depends on the distance of the test specimen from the chloride source (i.e., the tide line), showing that the more chlorides an environment contains, the more corrosive it will be.

The two values in bold type in Table 6.4-11 below are used in the calculations to determine the effect of Stainless Steel Type 316L ground support degradation upon crown seepage water (Section 6.8).

Table 6.4-11. Corrosion Rates of Stainless Steel Type 316L Under Various Environmental Conditions

Environment	Maximum ($\mu\text{m}/\text{year}$)	Mean ($\mu\text{m}/\text{year}$)	Minimum ($\mu\text{m}/\text{year}$)
100°C J-13 Steam ¹	0.099	0.099	0.099
150°C J-13 Steam ¹	0.064	0.064	0.064
Marine Atmosphere ¹	0.517	0.113 ^a	0.000
Industrial Atmosphere ¹	0.014	0.008	0.000
Rural Atmosphere ¹	0.00	0.00	0.00
207°C Brine Steam ¹	53	49.67	48
29.5°C Freshwater ²	0.0475	0.0083	0.0007
50°C Freshwater ²	0.2286	0.1614	0.1016
70°C Freshwater ²	0.2540	0.2413	0.2286
80°C Freshwater ²	0.2794	0.2141	0.1090
90°C Freshwater ²	0.2540	0.2032	0.1524
100°C Freshwater ²	0.5100	0.3247	0.0370
26.7°C Saltwater ²	14.787	1.939 ^a	0.0014

Sources: ¹ DTN: MO0312SPAPCEML.003 [DIRS 167409], *atmospheric.xls*.

² DTN: MO0409SPAACRWP.000 [DIRS 172059], *aqueous-316L.xls*.

NOTE: ^a This item's source, Table 4.1-1, are qualified for intended use in Appendix E, and calculated in output DTN: MO0407SPAPCEML.005.

6.4.1.6 Carbon and Low Alloy Steels

The corrosion rates for carbon and low alloy steels in different environments are shown in Table 6.4-15. Thus far, no specific data have been located for corrosion at 25°C of "A516", but the composition of Carbon Steel Type A516 is a carbon or low alloy steel (> 98 percent iron, Table 4.1-16) and it is considered equivalent to any other carbon/low alloy steel for corrosion purposes. Under subaerial exposure, the highest corrosion rate of 1,057.18 $\mu\text{m}/\text{year}$ comes from a steel sample sitting directly on the beach at Cape Kennedy, Florida. This sample was fully exposed to constant sea spray and is an indication of how salt buildup may affect the corrosion of metals. The lowest rate (0.4 $\mu\text{m}/\text{year}$) comes from a rural atmosphere at a relative humidity below 60 percent. These two values show how the corrosion rate for these steels can greatly differ depending on the atmospheric environment.

Aqueous corrosion rates of carbon and mild steels are much lower than marine or industrial atmospheric corrosion rates. Temperature effects are also different. In atmospheric corrosion, there is generally a direct correlation between temperature and corrosion rate. However, in aqueous environments, corrosion at 60°C is greater than that at 90°C. This is corroborated by Brasher and Mercer (1968 [DIRS 100883]), who measured the relationship between corrosion and temperature (Figure 6.4-2). As shown in the worksheet titled "rate vs. temperature" in DTN: MO0409SPAACRWP.000 [DIRS 172059], the highest corrosion rates occur at 60°C. The corrosion rate decreases with either increasing or decreasing temperature from this value (i.e., corrosion rates for 25°C and 90°C will be lower than the 60°C rates). As can be seen from Figure 6.4-2, the rates for the mild steel are within the same range as those for the Carbon Steel Type A516 as provided by McCright (1998 [DIRS 114637]). The data plotted in Figure 6.4-2 show that in corrosion for mild steel, the rates at 25°C are slightly lower than those at 90°C.

(Tables 6.4-12 through 6.4-14 intentionally deleted.)

Table 6.4-15. Corrosion Rates of Carbon and Low Alloy Steels in Various Environmental Conditions

Environment	Maximum ($\mu\text{m}/\text{year}$)	Mean ($\mu\text{m}/\text{year}$)	Minimum ($\mu\text{m}/\text{year}$)
60°C-SDW near 100% RH**	74.25	41.97	18.60
90°C-SDW near 100% RH**	135.26	63.60	22.69
60°C-SCW near 100% RH**	360.78	177.16	76.38
90°C-SCW near 100% RH ^a	423.06 ^a	195.44 ^a	72.96 ^a
Marine Atmosphere (80% relative humidity and over)**	851.09	153.33	9.87
Marine Atmosphere (70% to 80% relative humidity)**	1,057.18	101.94	6.39
Industrial Atmosphere (Over 80% relative humidity)**	123.00	102.5	85.50
Industrial Atmosphere (70% to 80% relative humidity)**	137.80	46.28	12.55
Industrial Atmosphere (60% to 70% relative humidity)**	164.54	20.58	3.77
Semi-Industrial Atmosphere (over 80% relative humidity)**	171.70	119.93	75.3
Semi-Industrial Atmosphere (60% to 70% relative humidity)**	60.88	35.23	17.33
Rural Atmosphere (over 80% relative humidity)**	60.10	39.19	21.60
Rural Atmosphere (70% to 79% relative humidity)**	59.00	26.63	10.68
Rural Atmosphere (60% to 69% relative humidity)**	75.50	19.37	3.93
Rural Atmosphere (less than 60% relative humidity)**	38.67	13.86	0.40
Urban Atmosphere (70% to 80% relative humidity)**	68.70	34.81	10.76
Urban Atmosphere (60% to 70% relative humidity)**	93.70	38.71	7.12
Urban Atmosphere (below 60% relative humidity)**	29.16	11.09	0.70
60°C-SDW*	106.93	77.43	65.77
90°C-SDW*	88.68	51.80	29.53
60°C-SCW*	14.36	10.61	6.77
90°C-SCW*	9.35	6.84	3.69

Sources: * DTN: MO0409SPAACRWP.000 [DIRS 172059], *aqueous-A516.xls*.**DTN: MO0312SPAPCEML.003 [DIRS 167409], *atmospheric.xls*, Tab "lab results (100%RH)."NOTE: ^a This item's source DTN: LL980704605924.035 is qualified for intended use in Appendix E and calculated in output DTN: MO0407SPAPCEML.005, *atmospheric.xls*, Tab "mild-structural-carbon steel."

Source: DTN: MO0409SPAACRWP.000 [DIRS 172059], *aqueous -- A516.xls*.

Figure 6.4-2. Corrosion Rates for Mild Steel in Water, Plotted as a Function of Temperature (°C)

6.4.2 Material Lifetimes

The expected lifetime of the introduced materials in the repository will be influenced by environmental parameters such as temperature, relative humidity, and available oxygen. Due to the variability of the in-drift environment, the corrosion rates are compiled into Table 6.4-18 by finding the maximum corrosion rate to represent each of the rate categories (maximum or 95%, mean or 50%, and minimum or 5%) for aqueous and atmospheric conditions. The "Comments" column in Table 6.4-18 indicates the conditions under which the corrosion occurred.

The materials that corrode away within a few hundred years (the low-alloy carbon steel) will consume oxygen with the greatest rate and form oxides that will settle in the drift. It is anticipated that the remaining materials will last long enough to potentially interact with crown seepage water entering the drift and to possibly influence the chemistry of those waters.

The long-lasting component most likely to interact with crown seepage is the stainless steel ground support along the crown of the drift, and this interaction is explicitly analyzed in Section 6.8 and found to have an insignificant impact on water chemistry.

The analysis in Section 6.8 uses the Stainless Steel Type 316L mean corrosion rates of 0.113 µm/year (steam and atmospheric) and 1.939 µm/year (fresh or salt water) from Table 6.4-18 as direct input for the abstraction of Stainless Steel Type 316L in Section 6.8.3. The availability of oxygen, as decreased by corrosion in the drift, is addressed in Section 6.7. The mean corrosion rate of 195.44 µm/year for carbon or low alloy steels (Table 6.4-18) is used as direct input for calculating the availability of oxygen in Section 6.7.

Table 6.4-18. Selected Corrosion Rates of Metallic and Alloy Materials for Use in Engineered Barrier System Chemical Environment Calculations

Material	Environmental Conditions	Maximum Corrosion $\mu\text{m}/\text{year}$	Mean or 50 th Percentile Corrosion $\mu\text{m}/\text{year}$	Minimum Corrosion $\mu\text{m}/\text{year}$	Reference	Comments
Titanium (Grade 16)	Water dripping case (seepage environment)	0.113	0.0237	0.00418	Table 6.4-2	50 th percentile corrosion used, not the mean
Alloy 22	25°C	0.0058	0.0024	0.0005	Table 6.4-3	50 th percentile corrosion used, not the mean
Alloy 22	100°C	0.0477	0.0193	0.0039	Table 6.4-3	50 th percentile corrosion used, not the mean.
Alloy 22	150°C	0.1278	0.0518	0.0104	Table 6.4-3	50 th percentile corrosion used, not the mean
Copper Alloy	Steam and atmospheric	6.6	4.79	3.15	Table 6.4-8	J-13 steam, 95°C to 100°C, near 100 relative humidity
Aluminum Alloy	Fresh/salt water	110.91	12.95	0.4	Table 6.4-9	Saltwater for maximum, fresh water for mean and minimum
Stainless Steel Type 316L	Steam and atmospheric	0.517	0.113 ^a	0.099	Table 6.4-11	Marine atm for maximum and mean and 100°C J13 steam for minimum (data for 207°C brine steam not included)
Stainless Steel Type 316L	Fresh/salt water	14.787	1.939 ^b	0.2286	Table 6.4-11	26.7°C saltwater for maximum and mean and 70°C fresh water for minimum
Carbon or Low Alloy Steels	Steam and atmospheric	1,057.18	195.44 ^a	85.5	Table 6.4-15	Maximum marine atm 70 to 80% RH, mean SCW 90°C steam, and minimum industrial atm. Over 80% RH
Carbon or Low Alloy Steels	Simulated water	106.93	77.43	65.77	Table 6.4-15	60°C SDW for all

Sources: DTN: MO0312SPAPCEML.003 (Indirect only, [DIRS 167409]) and MO0409SPAACRWP.000 [DIRS 172059]; only bolded items are used further as direct input. Source for titanium corrosion rates is BSC 2004 [DIRS 169845; Table 17]. Source for Alloy 22 corrosion rates is DTN: MO0409MWDUGCMW.000; [DIRS 171714] Base Case GC Rate CDF.xls; Tab: "Base Case GC Rate."

NOTES: ^a Item's source is qualified for modeling use (Appendix E); contained within the output DTN: MO0407SPAPCEML.005.

^b DTN: MO0409SPAACRWP.000 [DIRS 172059], aqueous-316L.xls, Tab "saltwater."

^c Values in the 3rd, 4th, and 5th columns are means unless specified as 50th percentiles in the Comments column.

Figure 6.4-3 shows the mean (or 50th percentile), minimum, and maximum lifetimes of materials listed in Table 6.4-18. These material lifetimes are presented on a per centimeter basis as that distance is an excellent proxy for general material thickness, within an order of magnitude. Specifically, material lifetimes were hand calculated by dividing 10,000 $\mu\text{m}/\text{cm}$ conversion by the mean or 50th percentile, minimum, and maximum corrosion rates ($\mu\text{m}/\text{year}$) for each material given in Table 6.4-18. For example, the minimum corrosion rate for titanium (Grade 16) given in Table 6.4-18 is 0.00418 $\mu\text{m}/\text{year}$, thus by dividing 10,000 $\mu\text{m}/\text{cm}$ by 0.00418 $\mu\text{m}/\text{year}$, the maximum lifetime for titanium is calculated to be approximately 2.392×10^6 yr/cm of material.

Figure 6.4-3. Relative Material Lifetimes Using the Mean or 50th Percentile, Minimum, and Maximum Corrosion Rates from Table 6.4-18.

As can be seen by Figure 6.4-3, the mean lifetime values for carbon or low-alloy steels in a steam and atmospheric environment is over one order of magnitude less than any other material. This comparison leads to the conclusion that for modeling of oxygen consumption, due to and proportional to corrosion, the most significant consumption from low-alloy or carbon steels will lead to a reasonable approximation of the total oxygen demand. The oxygen balance calculation based upon this is performed in Section 6.7.1.

6.5 GEOCHEMICAL MODELING CONSTRAINTS

This section summarizes the main set of mathematical models used in this report and establishes a modeling framework for developing equilibrium-type geochemical models in systems under metastable or partial equilibrium. This section can be thought of as a supplement to the conceptual model outlined in Section 6.2. It is also intended to demonstrate the importance of mineral and species suppression (i.e., the way equilibrium models are used to predict chemical conditions in metastable systems), which is a fundamental modeling concept of this model report. Some sensitivity studies discussing the uncertainties associated with this concept are further evaluated in Section 6.12.4.

6.5.1 Mathematical Models Implemented by the Use of EQ3/6 V8.0 Geochemical Modeling Software

Geochemical modeling constraints are imposed by the primary geochemical modeling software used in this report, *EQ3/6 Version 8.0* (STN: 10813-8.0-00 [DIRS 162228]). This software is composed of two independent codes: EQ3NR and EQ6. Both of these are described in general terms in the following subsections, much of which is derived from *Software User's Manual EQ3/6 Version 8.0* (SNL 2003 [DIRS 162494], Appendices B and D). The reader is referred to the EQ3/6 software users manual for a more detailed explanation of the concepts discussed in the following paragraphs.

6.5.1.1 EQ3NR: Speciation-Solubility Modeling of Aqueous Systems

EQ3NR is an equilibrium speciation-solubility code for aqueous systems. As such, given sufficient data for a chemical species to characterize a specific aqueous system, it computes a model of the solution that consists of two principal parts: the distribution of species in the solution and a set of saturation indices ($SI = \log Q/K$) for various reactions of interest. The saturation indices measure the degree of disequilibrium of corresponding solution-mineral reactions. They provide a means for evaluating solubility controls on natural waters. For example, at equilibrium the $SI = 0$, but under close to equilibrium conditions where a series of related fluids all have a given mineral SI value close to zero, it is probable that this mineral is present and partial equilibrium with this mineral is maintained as the solutions evolve in composition.

EQ3NR is not a specific computerized geochemical model, but a software code that is useful in evaluating many different conceptual geochemical models, which are defined by the contents of a supporting data file (from which there are now several to choose from, including *Data0.ymp.R2* and *Data0.yfp*) and by other user-defined inputs and constraints in the EQ3NR input file. The supporting data files differ not only in terms of data values, but also, more importantly, in terms of the identities of the components and chemical species represented, and in terms of the general approaches used in the estimation of activity coefficients. Because of various limitations (such as the use of the Pitzer model for estimation of activity coefficients), some problems may require the use of only certain data files, while others can be treated using any of the available data files.

Although speciation-solubility models are commonly used as a means of testing whether heterogeneous reactions are in a state of thermodynamic equilibrium, they often just assume that all reactions occurring in aqueous solution are in such a state. Reactions most likely to be in disequilibrium are redox reactions or reactions for the formation or dissociation of large complexes that are more like small polymers, such as $(\text{UO}_2)_3(\text{OH})_7^-$. Speciation-solubility models are better used when they are employed to test the degree of disequilibrium of these kinds of reactions than when these are assumed to be in equilibrium.

An equilibrium speciation-solubility model cannot, by itself, predict how aqueous solution composition will change in response to rock-water interactions. Nevertheless, this type of modeling can be a powerful tool for elucidating such interactions when it is applied to a family of related waters. Such a family might be a set of spring waters issuing from the same geologic formation, a sequence of groundwater samples taken along an underground flow path, or a sequence of water samples taken in the course of a rock-water interactions experiment in the laboratory. Jenne (1981 [DIRS 162479]) reviews several studies of this kind. Particularly interesting are the Nordstrom and Jenne (1977 [DIRS 162480]) study of fluorite solubility equilibria in geothermal waters and the Nordstrom et al. (1979 [DIRS 162508]) study of controls on the concentration of iron in acid mine waters. EQ3NR offers many options for the input file description of a given water chemistry's composition. Consequently, the code can be used in a variety of ways.

Many of the descriptive parameters of interest can be either model inputs or outputs. For example, the pH of a buffer solution can be calculated from the buffer recipe by adjusting the hydrogen ion concentration to satisfy charge balance. Alternatively, adjusting the concentration of a buffer component to satisfy the charge balance is a means of computing the complete recipe for a buffer having a desired pH. Some possible model inputs may be constraints, as in specifying equilibrium with one or more specified mineral phases.

6.5.1.1.1 Input Constraints, Governing Equations, and Outputs

Aqueous speciation models can be constructed to satisfy a variety of combinations of possible input constraints and governing equations. The input constraints may include:

- Total (analytical) concentrations
- An electrical balance requirement
- Mass balance
- Free ion concentrations
- Aqueous species activities
- pH
- Eh
- pe
- Oxygen fugacity
- Phase equilibrium requirements
- Homogeneous equilibria
- Run-specific values for equilibrium constants.

The governing equations are the corresponding mathematical expressions, such as the mass balance equation and the charge balance equation.

The choice of governing equations in large part depends on which parameters are to be inputs to the model, and which are to be outputs. This, in turn, is a function of what data on a given water are available, what form they are in, and what constraints the modeler would like to use.

Chemical analysis mainly provides a set of values for the so-called total concentrations of dissolved components. The analytical value for an ion such as calcium is an example. It does not discriminate between the various calcium species in solution, but rather estimates the dissolved calcium contributed by all of them. This leads to a mass balance equation of the form:

$$m_{T,Ca} = m_{Ca^{2+}} + m_{CaOH^{-1}} + m_{CaCO_{3(aq)}} + m_{CaHCO_3^+} + \dots \quad (\text{Eq. 6.5-1})$$

where $m_{T,Ca}$ is the total or analytical concentration (on the molal scale) and m_i is the molality of any individual chemical species contributing to the mass balance. The summations must be weighted by the appropriate stoichiometric equivalences; for example, in the case of F:

$$m_{T,F} = m_{F^-} + m_{HF_{(aq)}} + 2m_{H_2F_{2(aq)}} + 2m_{HF_2^-} + 3m_{AlF_{3(aq)}} + \dots \quad (\text{Eq. 6.5-2})$$

The total concentration is the most common type of input parameter to an aqueous speciation model. Therefore, the most common governing equation is the mass balance constraint. As will be seen, there are situations in which a total concentration is replaced by another type of input such as the use of the input flag "heterogeneous equilibrium" where an aqueous concentration can be calculated from a gas fugacity. In these cases, the mass-balance constraint is replaced by a different governing equation, and the total concentration becomes something to be calculated (an output parameter). Charge balance is also a common governing concept that will either calculate the apparent charge imbalance or force the aqueous solution to maintain electrical balance. Large charge imbalance errors indicate there may be incomplete or erroneous chemical analysis or a misinterpretation of reported analytical results.

Mathematically, there is no reason to discriminate among ion pairs (and ion triplets, etc.) and complexes. For some investigators, the term "ion pair" implies a species in which an anion is separated from a cation by an unbroken hydration sheath about the latter, whereas the term "complex" implies direct contact and perhaps some degree of covalent bonding. Other investigators use these terms interchangeably. It is a general presumption in cases of geochemical interest that the concentrations of ion pairs and complexes are governed by thermodynamic equilibrium.

Each case of this equilibrium can be represented by a mass-action equation for the dissociation of the ion pair or complex. As an example, the calcium sulfate ion pair dissociates according to the reaction:

where “=” is used as the sign for a reversible chemical reaction. The corresponding mass-action equation is:

$$K_{CaSO_4(aq)} = \frac{a_{Ca^{2+}} a_{SO_4^{2-}}}{a_{CaSO_4(aq)}} \quad (\text{Eq. 6.5-4})$$

where K is the equilibrium constant and a_i represents the thermodynamic activity of each species. This may also be written in logarithmic form:

$$\log K_{CaSO_4(aq)} = \log a_{Ca^{2+}} + \log a_{SO_4^{2-}} - \log a_{CaSO_4(aq)} \quad (\text{Eq. 6.5-5})$$

The thermodynamic activity is related to the molal concentration by the relation:

$$a_i = m_i \gamma_i \quad (\text{Eq. 6.5-6})$$

where γ_i is the activity coefficient, a function of the composition of the aqueous solution. As the solution approaches infinite dilution, the value of γ_i for each species approaches unity. The user, in the EQ3/6 input calculation file, chooses the set of equations for computing the activity coefficients of aqueous species. The requisite supporting data are on the EQ3/6 database file. The activity of pure mineral phases is specified to be at unity.

6.5.1.1.2 Activity Coefficient Models of Aqueous Species

The thermodynamic activities (a_i) of aqueous solute species are usually defined on the basis of molalities. Thus, they can be described by the product of their molal concentrations (m_i) and molal activity coefficients (γ_i), as shown in Equation 6.5-6.

The thermodynamic activity of the water (a_w) is always defined on a mole fraction basis. Thus, it can be described analogously by the product of the mole fraction of water (x_w) and its mole fraction activity coefficient (λ_w):

$$a_w = x_w \lambda_w \quad (\text{Eq. 6.5-7})$$

The activity coefficients, in reality, are complex functions of the composition of the aqueous solution. In electrolyte solutions, the activity coefficients are influenced mainly by electrical interactions. Much of their behavior can be correlated in terms of the ionic strength, defined by:

$$I = \frac{1}{2} \sum_i m_i z_i^2 \quad (\text{Eq. 6.5-8})$$

where the summation is over all aqueous solute species and z_i is the electrical charge. However, the use of the ionic strength as a means of correlating and predicting activity coefficients has a very limited range of usefulness (e.g., in the mean salt method of Garrels and Christ (1965 [DIRS 144877], pp. 58 to 60)). A comparison between the mean salt method of Garrels and

Christ and Debye-Hückel (1965 [DIRS 144877], Fig 2.15, p. 63) shows a reasonable agreement up to an ionic strength 0.05 to 0.1 depending on the ion. In general, model equations that express the dependence of activity coefficients on solution composition only in terms of the ionic strength are restricted in applicability to dilute solutions.

The three basic options for computing the activity coefficients of aqueous species in EQ3/6 calculations are models based on the Davies (1962 [DIRS 162482]) equation, the Hückel equation, also known as the “B-dot” equation (Helgeson 1969 [DIRS 137246]), and Pitzer’s equations (1973 [DIRS 152738]; 1975 [DIRS 152740]; 1979 [DIRS 119530]; 1987 [DIRS 162481]). The first two models, owing to limitations on accuracy, are only useful in dilute solutions (generally up to ionic strengths of 1 molal, although extension for specific application is possible). The third basic model is useful in highly concentrated as well as dilute solutions, but is limited in terms of the components that can be accurately treated, as defined by the input database. Calculations of relevance to this report were performed with either B-dot or Pitzer activity models.

With regard to temperature and pressure dependence, all of the following models are parameterized along the standard EQ3/6 curve, which is 1.013 bar up to 100°C and the steam-liquid water equilibrium curve at higher temperatures.

All EQ3/6 calculations in this report, with the exception of the calculations performed in Section 6.8, use the Pitzer activity model, the usual formulation of which implies (in the absence of other action) a nonstandard “Pitzer” pH scale. However, the results of this report are presented in terms of National Bureau of Standards pH. The primary users of the output of this model are using its calculated pH values to represent input parameters to models established on laboratory measurements using National Bureau of Standards pH standards. The same measurement standard is true for values of pH input into EQ3/6 calculations (if a scale for pH output is chosen, any pH input is thought to be on the same scale). This pH scale conversion is done internal to EQ3/6 software following the discussion outlined in *Software User’s Manual EQ3/6 Version 8.0* (SNL 2003 [DIRS 162494], Attachment B, Equation B-99).

6.5.1.2 EQ6: Reaction-Path and Single-Point Modeling

EQ6 computations can first be broken down into “single-point” thermodynamic equilibrium calculations and irreversible mass transfer reaction-path calculations. A single-point thermodynamic calculation is essentially just the special case of a reaction path with no steps (e.g., used when precipitating supersaturated phases or making a temperature jump). Reaction paths may be calculated for titrations, irreversible reaction in closed systems, and irreversible reaction in certain well-defined types of open systems (e.g., a fluid-centered flow-through open system). Such calculations may be in reaction progress mode (time independent) or time mode (explicit kinetic or time dependent), depending on the rate law being implemented.

EQ6, uses separate methodologies for treating intrinsically algebraic equations and intrinsically differential equations. The former govern the thermodynamic calculations, and the latter are comprised of rate laws for irreversible processes. This numerical decoupling makes it possible to perform thermodynamic calculations, given the necessary inputs of total number of moles of components, the temperature, and the pressure, independently of the integration of rate

equations. This decoupling permits making “single-point” thermodynamic equilibrium calculations, such as temperature jump problems, in which rate equations do not appear.

In EQ6 reaction-path models, the two types of equations are coupled in the mathematically formal sense, but the solution of each is performed semi-independently. Each calculation type is performed alternately, the output of one becoming the input to the next execution of the other. For example, in moving a step forward in reaction progress (ξ), rate equations are integrated. This defines new values for the temperature, pressure, and total number of moles of the components, which are inputs to the following thermodynamic calculation. This, in turn, gives a new distribution of species from which values may be calculated for the rates of the irreversible processes at the new point. If accuracy tests on the ordinary differential equation integration are satisfied, these rate values are used in making the next integration step. Otherwise, the step size may be cut until those tests are satisfied.

When the rate chosen to constrain an irreversible process is a relative rate ($d\xi_j/d\xi$), the rate function is either a constant or a simple function of the overall reaction progress variable (ξ). When EQ6 operates in the mode of arbitrary kinetics (all irreversible processes constrained by relative rate expressions; no time variable in the model), these rates can be integrated by simple closed-form expressions. It is, therefore, possible to take arbitrarily large step sizes, subject only to the following conditions.

In the case of closed and open system calculations, the rate of an irreversible reaction is set to zero when the corresponding thermodynamic driving force, the affinity, is no longer positive. Affinities are outputs of the thermodynamic calculations. EQ6 locates the point of reaction progress where the affinity goes to zero. If the corresponding reactant is a mineral, this means that the aqueous solution has reached saturation. The code then changes the status of the reactant to inactive (meaning it is effectively removed from the set of reactants) and any remaining mass of the reactant is moved into the *equilibrium system*. Titration calculations are very similar to closed-system calculations, but the rate of an irreversible reaction is not set to zero when saturation is reached, and the remaining reactant mass continues to be added to the equilibrium system according to the rate law.

The rate of an irreversible reaction rate also becomes zero when the associated “reactant” becomes exhausted, no matter what kind of system model the code is dealing with. The user specifies how much of a reactant is available at the start of the calculation run. The code then finds the point of reaction progress at which exhaustion occurs.

6.5.1.2.1 Constraints on Thermodynamic Calculations

The following thermodynamic constraints are enforced in EQ6 calculations:

- Mass balance
- Charge balance
- Law of mass action
- Activity coefficients of aqueous species
- Activity coefficients of solid solution components
- Saturation indices and affinities.

Details on each of these can be found in *Software User's Manual EQ3/6 Version 8.0* (SNL 2003 [DIRS 162494], Appendix D1.2).

6.5.1.2.2 Constraints on Reaction Path Calculations

The following reaction path constraints are enforced in EQ6 calculations:

- Reaction progress variable (ξ), which is a measure of the extent to which a reaction has proceeded
- Reaction rates and time for each irreversible reaction as a function for either the relative rate or the absolute rate
- Rate laws programmed into EQ6: relative rate, partial equilibrium, transition-state theory, and linear rate.

Details on each of these can be found in *Software User's Manual EQ3/6 Version 8.0* (SNL 2003 [DIRS 162494], Appendix D1.3).

6.5.2 Geochemical Modeling Methodology

Generally, a reaction path geochemical equilibrium model is constructed using the steps outlined in Figure 6.5-1. First, a conceptual model is defined where the chemical system and state are defined. This system and state are tested and investigated to produce results. Those results are compared with independent experimental, natural analog, or other modeling data to ensure that the model is representative of the system and state to be analyzed.

Decisions about mineral suppression or inclusion require:

- A reasonable understanding of mineralogy and petrology
- A well-researched conceptual model
- An understanding of how to develop a reaction-path model using software codes like EQ3/6 (Wolery 1992 [DIRS 100836]; Wolery and Daveler 1992 [DIRS 100097]), PHREEQC (Parkhurst 1995 [DIRS 142177]), or MINTEQA2 (HydroGeoLogic and Allison Geoscience Consultants 1999 [DIRS 158974])
- An understanding of how to ensure that confidence exists in the model and that model uncertainty has been appropriately addressed.

The following subsection contains a brief summary of the kinetics versus equilibrium relations rationale that must be considered in the selection of mineral phases for the model. Bethke (1996 [DIRS 162270]), Smith and Missen (1991 [DIRS 161602]), and Van Zeggeren and Storey (1970 [DIRS 161603]) provide more-detailed discussions concerning modeling methodology aspects.

6.5.3 Equilibrium Versus Kinetics

Bethke (1996 [DIRS 162270], Chapter 2) reports there are two main types of equilibrium end states that are important to recognize in reaction path modeling: complete and metastable equilibrium. In complete equilibrium, the chemical state of the system attains stable equilibrium such that there is no chemical potential to drive any net chemical reaction. Usually, when an equilibrium model is first constructed, the first-order model (Figure 6.5-1) is allowed to go to complete equilibrium. When the initial system is constrained based on the end equilibrium state by determining variables such as the temperature, dissolved aqueous concentrations, quantity of given minerals in the system, or the fugacities of any gases, the calculation results in a fluid saturated with respect to the stable equilibrium mineral assemblage for the system.

Once this first-order model is constructed, the boundary conditions and the conceptual model are evaluated to determine whether various states of metastable equilibrium should be taken into account (Section 6.5.5). The first-order model is then refined to account for these effects. For example, if the model predicts the complete equilibrium state to include minerals that do not occur in the actual system, this may imply that a metastable equilibrium situation exists in the actual system.

Metastable equilibrium occurs when one or more chemical reactions proceed toward equilibrium at a rate that is so small on the time scale of interest that the system does not reflect the consequences of reaction with that phase. In this case, the system can be considered not to include the reaction(s) involving that mineral. Such reactions are commonly heterogeneous reactions involving mineral precipitation. That is, the nucleation or growth of the mineral is subject to kinetic barriers that are large enough to preclude, or allow only negligible progress of, the reaction. In such a case, the mineral that should exert an equilibrium compositional constraint is supplanted by another, less stable, phase that is not kinetically constrained from forming and growing.

In other words, mineral suppression is used in equilibrium calculations to represent, in a simple manner, the fact that some solid phases are kinetically inhibited from precipitating or dissolving under equilibrium conditions in certain environments (e.g., quartz precipitation at low temperature). Because of the kinetic constraints, the chemical constituents commonly controlled by the inhibited solid phase are controlled instead, if at all, by a somewhat less-stable phase that reaches its metastable equilibrium rapidly compared to the inhibited phase. Inclusion of the explicit kinetic approaches would handle mineral dissolution or precipitation directly, but for simpler equilibrium calculations this is commonly handled by suppressing the occurrence of that phase in the model to represent the kinetic barrier and to achieve the same result found in real systems. Suppression of minerals, therefore, is a practical tool in being able to define the end-state equilibrium of a modeled system or to use an equilibrium-type model to mimic the effect of kinetic processes without having to know actual details about the kinetic rates of dissolution or precipitation.

The Process Required to Give a Valid Technical Basis for Mineral Suppression or Inclusion

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NOTE: A first order model is a model that accounts for complete equilibrium (i.e., no metastable equilibrium or kinetic controls) with no active mineral suppressions.

Figure 6.5-1 A Simplified Roadmap of the Process Required to Give a Valid Technical Basis for Mineral Suppression or Inclusion in Geochemical Equilibrium Modeling

Partial equilibrium and local equilibrium are specific cases or subsets of metastable equilibrium that can have relevance to a given geochemical problem. Partial equilibrium (also known as heterogeneous equilibrium) is defined by Wolery and Daveler (1992 [DIRS 100097]) in that some (usually most) reactions are in a state of equilibrium, while others, usually few in number and representing heterogeneous processes such as mineral dissolution or precipitation, are not.

For example, the fluid in sandstone might be in equilibrium itself but may not be in equilibrium with the mineral grains in the sandstone or with just some of the grains. Local equilibrium, which is sometimes called mosaic equilibrium (i.e., temperature, mineralogy, or fluid chemistry vary across the system of interest), can be thought of as a system that is open to groundwater flow (Bethke 1996 [DIRS 162270], p. 12). In this idealized flow through system, the aqueous phase moves over or through several different mineral assemblages and the water reacts with each of these and achieves some degree of equilibrium on the local scale with each assemblage, even though each location is at a different equilibrium state comparatively. All of these various types of equilibrium conditions can be combined into a single model, depending on the conceptual model.

Kinetics can be combined into reaction path modeling because the equilibrium point of a reaction is the point at which dissolution and precipitation rates balance. Bethke (1996 [DIRS 162270], Chapter 2) indicates that kinetic reactions fall into three groups:

- Those in which reaction rates are so slow relative to the period of interest that the reaction can be ignored (i.e., accounting for metastable equilibrium). This slow reaction rate group commonly corresponds to what mineral suppression is used to represent.
- Those fast enough to maintain equilibrium (accounting for complete equilibrium)
- All other reactions that do not fall into the first two groups. These "...other reactions" are the only reactions that require a kinetic description.

6.5.4 Engineered Barrier System Geochemical Equilibrium Modeling

The equilibrium reaction path models used by the physical and chemical environment model are designed to predict long-term chemical processes within a potential repository drift. Although short-term occurrences (such as seepage water falling onto the drip shield) can cause transitory divergence from the conceptualized state of metastable equilibrium, an equilibrium approach is adopted because it provides valuable insight into long-term processes. This modeling provides the exposure conditions needed by *General Corrosion and Localized Corrosion of Waste Package Outer Barrier* (BSC 2004 [DIRS 169984], Section 6.4.4), specifically these are pH, and chloride and nitrate ion concentrations.

An equilibrium reaction-path model, such as that implemented using the EQ6 software, relies on a thermodynamic database that contains standard-state thermochemical parameters of the different chemical species in a system to determine the chemical reaction equilibria as functions of the changing conditions. In addition to the homogeneous reactions that occur within each phase (e.g., water, gas, solid), there are heterogeneous reactions that involve more than one phase, such as mineral precipitation and degassing of volatile constituents from the aqueous phase. Most of the reactions in the equilibrium models employed by the engineered barrier system physical and chemical environment model are rapid relative to the timeframe of the modeling period; therefore, most reactions are allowed to reach equilibrium. However, there are many minerals in the thermodynamic database that will not form under the expected conditions of the repository. These minerals predominantly include those that require high pressures or very high temperatures to achieve the kinetic rates of formation that would produce a significant

mass within the modeling time frame. Other minerals that could be excluded from consideration are those that form during the oxidation of pyrite or other sulfide minerals, which form only under redox conditions that will not occur in the repository (Section 6.7.1).

The pressure in the repository is expected to remain near atmospheric, and the temperature at the drift wall is not expected to rise above 200°C (Figure 6.7-7). These conditions limit those minerals in the database that can realistically be expected to form at a significant rate. As discussed previously, an equilibrium model ignores the use of kinetic rates; it predicts the most stable mineral phases at equilibrium, except when the user suppresses (i.e., rules out) those minerals. When precipitation is suppressed for a mineral, the equilibrium model does not allow the mineral to precipitate, resulting in a condition of supersaturation with respect to that phase. In this way, the equilibrium model can incorporate simplified kinetic constraints as metastable equilibrium conditions. Current conceptualization of postclosure drift conditions allows for conditions in the repository to be essentially dry. Any seepage entering the drift would be subject to conditions in which the relative humidity or activity of water would fall below one. Therefore, evaporative processes are expected to dominate during the evolution of in-drift seepage.

6.5.4.1 Modeling of Mineral Precipitation

The Pitzer thermodynamic database (*Data0.ypp*) currently includes more than 220 minerals, but only a small fraction of these have been suppressed in the modeling run calculations evaluated to date. It is unnecessary to identify *a priori* which of the more than 220 minerals should be suppressed for these calculations. The limited range of chemical compositions of the waters likely to occur within the drift dictates that a majority of the more than 220 minerals will never achieve a chemical potential favoring precipitation. This point is demonstrated by the results to date. So far, over 368 different observed and predicted water compositions at Yucca Mountain have been evaporated to dryness using Version 8.0 of the EQ3/6 software and the new Pitzer database (Section 6.6), yet fewer than 40 minerals have become saturated or supersaturated with respect to the aqueous composition. Thus, it is not necessary to categorize the remaining 180-plus minerals according to their potential for precipitating under drift conditions.

Having some sort of simple criteria to appropriately suppress or include the approximately 40 minerals that have become saturated in the engineered barrier system models being developed for TSPA-LA facilitates determining the end equilibrium state in a model. Six criteria have been developed to assist in determining the rationale for suppression or inclusion in the models to account for the kinetic or metastable equilibrium arguments stated previously. These six criteria are listed in the following paragraphs.

Criterion 1—Is the mineral of interest beyond or outside the defined chemical system of the model?

If the mineral lies outside or beyond the defined chemical system of the model, there is no reason to include the mineral. For example, while modeling mineral formation at low temperatures and pressures (near ambient), any mineral could be excluded that was known to form only at high temperatures or pressures.

Individuals trained in mineralogy or petrology can readily make these determinations. Example reference sources, used to make these decisions when combined with expert judgment, are Klein and Hurlbut's *Manual of Mineralogy* (1985 [DIRS 105907]), Kerr's *Optical Mineralogy* (1977 [DIRS 161606]), and Roberts et al.'s *Encyclopedia of Minerals, 2nd Ed.* (1990 [DIRS 107105]), or any similar reference source that discusses the petrology or mineralogy of a given system or analogue system.

If a mineral is not included in the database, it is, in effect, suppressed. The formation conditions applicable to the great majority of the over 3,000 minerals listed by Roberts et al. (1990 [DIRS 107105]), lie outside the physiochemical boundaries of the repository system. Most of these can be excluded because they contain trace or minor elements of no interest to repository operations, or have been addressed through studies of corrosion and radionuclide solubility. Table D-1 in Appendix D provides details on an additional 709 minerals that are not in *data0.ympr.R2* or *data0.yppf*; these minerals are not included in the current modeling effort for various reasons as detailed in Table D-1.

Criterion 2—Is the mineral of interest likely or unlikely to precipitate because of kinetic controls?

Langmuir (1997 [DIRS 100051]) provides a general rule of thumb for determining the need for a kinetic description of mineral dissolution or precipitation. When a reaction is irreversible or its rate is comparable to, or slower than, the system residence time (i.e., the half-life is greater than or equal to the residence time), a kinetic rate is needed to describe the state of reaction. When this rule of thumb is met and kinetic data are available, the data are used directly. Often however, rate data are not available for the system being modeled, or it is much simpler to invoke a state of metastable equilibrium and use a mineral suppression to simplify the model. Therefore, a modeler will make a mineral suppression that mimics the conceptualized state of metastable or localized equilibrium. As an example, one of the most common mineral suppressions used in geochemical modeling is that of considering the kinetic rates of reaction for amorphous silica, quartz, or one of its polymorphs (tridymite and chalcedony). In general, amorphous precipitates will tend to form first, and then a process of mineral recrystallization will take place (Langmuir 1997 [DIRS 100051], p. 55). Therefore, the metastable phase that would generally be used in a reaction path model for quartz would be amorphous silica. If the conceptual model were to account for a longer system residence time or higher temperatures, the modeler would allow quartz or one of its polymorphs to precipitate. For iron oxides, it would be expected that either goethite or ferrihydrite would form first, depending on temperature and relative humidity. Ferrihydrite recrystallizes relatively quickly to form goethite or hematite, which may persist for eons.

Criterion 3—Is analytical or natural analog information available that warrants the inclusion or exclusion of the mineral?

Commonly, when performing geochemical modeling, information or data is found by researching the relevant literature used to develop the conceptual model. This information often comes from analytical data or natural analog information, and warrants the suppression or inclusion of minerals that could be dispositioned differently based on Criteria 1 and 2. This

allows for inclusion of minerals that could form due to some unknown kinetic constraint that has not been accounted for directly in the model.

Although care is taken in constructing and attempting to “validate” a model as it is developed, conceptual model or thermodynamic database uncertainty must still be addressed. Therefore, three additional criteria are included to allow evaluation of the effect of mineral suppressions on model results.

Criterion 4—Do minerals need to be suppressed or included to test overall model uncertainty or sensitivity due to reported uncertainty in the supporting literature, database, or conceptual model?

Criterion 5—Does the suppression or inclusion of minerals that are highly uncertain drive the resulting chemical output to a more or less conservative modeling result?

Criterion 6—Do other minerals that are in a database provide an adequate surrogate or proxy for the mineral?

Certainly, Criteria 4 through 6 are not the normal types of mineral dispositions in models. However, they are of great use when conducting sensitivity studies or handling modeling uncertainties.

Although the six criteria are written to address mineral suppressions, they can and should be used to document the suppression of any aqueous species of concern (Table 6.8-4).

6.5.4.2 Modeling of Trace Elements

The term “trace” used in reference to solutes in natural water cannot be precisely defined. Commonly, the term is used for substances that occur in concentrations less than 1.0 mg/L (Hem 1985 [DIRS 115670], pp. 129 to 130). Trace elements from the natural system that are potentially present in the in-drift seepage waters that have been identified and considered for affects on the waste package and drip shield environments are lead (Pb), arsenic (As), and mercury (Hg). The chemical composition of the rhyolite tuff that makes up the repository horizon is well characterized and essentially uniform (Peterman and Cloke 2002 [DIRS 162576]). Compositions of porewaters extracted from the tuff at the repository horizon have been characterized for trace element concentration. Table 6.5-1 shows the composition of selected minor and trace elements in the porewaters extracted from cores collected in the enhanced characterization of the repository block cross drift. As can be seen from Table 6.5-1, Pb and Hg concentrations and more than one third of the arsenic concentrations are below the detection limits.

Fluoride, trace elements in seepage, and elements in introduced materials that are normally considered as trace species in natural waters may be important to certain in-drift processes, yet not be significant contributors to the major ion geochemistry. Most analyses presented to date have focused on the chemical reactions among major constituents because these are considered to be the primary system drivers controlling the in-drift environmental conditions. Bruno et al. 1998 [DIRS 110969] also conclude in their studies of trace metals in natural systems that good characterization of the site mineralogy and a sound understanding of the main geochemical

driving forces (i.e., bulk chemistry) are needed to further investigate the reactions of trace species; that is, the trace species will only have a small effect upon the bulk chemistry (e.g., pH, ionic strength, or major cation-anion concentrations).

Fluoride and bromide are explicitly included in the analyses and discussions of Sections 6.6, 6.12, and 6.13. The potential impacts of fluoride on corrosion processes have also been evaluated and found to not significantly enhance the general corrosion of the drip shield under repository conditions (BSC 2004 [DIRS 169845], Section 8.3). Chromium and iron, considered major constituents of introduced materials in the drift, and trace element bromide in the seepage waters entering the drift, are specifically considered in Sections 6.8 and 6.12.4.3, respectively.

6.5.5 Rationale for Including or Excluding Precipitating Minerals

Table 6.5-2 provides a listing of the minerals that have been suppressed in the engineered barrier system in-drift precipitates/salts and physical and chemical environment models; Table 6.5-3 provides a listing of the minerals that precipitated during modeling run calculations. In each case, a rationale for the decision to suppress or include each mineral is provided. In addition to the rationale listed in Tables 6.5-2 and 6.5-3, which are used to strengthen model validation, each engineered barrier system model is independently validated against natural analog data or experimental results, to ensure that the model is an appropriate representation. Minerals that are present in the thermodynamic database but did not precipitate during model development were not included on Table 6.5-3.

Relevant natural analogs for the in-drift precipitates/salts and physical and chemical environment conceptual models are saline lakes and playa deposits; the evaporite mineral assemblages that form in those environments are documented by Eugster and Hardie (1978 [DIRS 100743]) and Papke (1976 [DIRS 162274]). These minerals should reflect the mineral assemblages that could form in the low-temperature, low-pressure, in-drift environment; where the activity of water is below one and the solution compositions are comparable. These analogs are used, in conjunction with the model boundary conditions in the low-temperature, low-pressure, in-drift environment, to strengthen the mineral suppression and inclusion rationale listed in Tables 6.5-2 and 6.5-3.

Table 6.5-1. Compositions of Fluoride and Trace Elements in Enhanced Characterization of the Repository Block Porewater Samples

Sample Designation	F	Br	Mn	Co	Zn	Rb	Sr	As	Mo	Ba	Hg	Pb	U
ECRB-SYS-CS400/3.8-4.3/UC	3.7	<1	410	<2.5	<100	41	3,580	8	13	420	<1.0	<2.0	6.9
ECRB-SYS-CS400/5.6-6.2/UC	1.7	<1	43	<2.5	<100	30	1,480	<6.0	4.8	<30	<1.0	<2.0	<0.3
ECRB-SYS-CS600/3.6-4.0/UC	2	<1	39	<2.5	<100	16	1,750	<6.0	5.3	<30	<1.0	<2.0	0.5
ECRB-SYS-CS1000/7.3-7.7/UC	3.4	<1	23	<2.5	<100	21	1,040	<6.0	5.3	<30	<1.0	<2.0	0.8
ECRB-SYS-CS750/6.2-6.5/UC	1.2	<1	54	<2.5	<100	22	1,160	<6.0	6.2	<30	<1.0	<2.0	10.3
ECRB-SYS-CS2150/5.5-6.1/UC	5.3	<0.2	38	<1.3	<100	16	1,110	5.7	8.9	<15	<1.0	<1.0	4.1
ECRB-SYS-CS900/5.4-5.9/UC	1.7	<0.2	77	<1.3	<100	12	1,980	5.4	7.4	<15	<1.0	<1.0	0.3
ECRB-SYS-CS850/5.1-5.6/UC	2.9	<0.2	14	<1.3	<100	9.3	1,150	8.3	13	<15	<1.0	<1.0	2.7
ECRB-SYS-CS900/3.5-4.1/UC	2	0.3	470	1.1	<50	20	4,090	3.4	9.5	<15	<1.0	<1.0	1.2
ECRB-SYS-CS1000/12.9-14.0/UC	2	<0.1	47	<1.0	<40	24	1,110	5.4	11	61	<1.0	<1.0	6.9
ECRB-SYS-CS450/5.3-6.0/UC	1.1	0.4	100	<1.0	40	32	1,240	5.7	5.1	46	<1.0	<1.0	0.1
ECRB-SYS-CS2300/4.3-4.9/UC	1.7	<0.1	260	<2.5	<100	22	590	<6.0	14	29	<1.0	<2.0	7.6
ECRB-SYS-CS500/12.0-16.7/UC	4.8	0.4	26	<2.5	<100	20	1,100	7.6	14	<30	<1.0	<2.0	2.5
ECRB-SYS-CS2000/16.5-21.1/UC	11	<0.2	58	<1.3	<100	33	1,390	5.9	22	<20	<1.0	<1.0	22.7
ECRB-SYS-CS2000/16.3-16.5/UC	6	<0.2	130	<1.3	<100	22	1,260	<3.0	22	<15	1.2 [1]	<1.0	11.3
ECRB-SYS-CS950/5.2-5.3/UC	1.9	<0.2	62	<1.8	<100	10	1,240	4	3.4	<25	<1.0	<1.6	<0.2
ECRB-SYS-CS950/4.8-5.5/UC	4.9	<0.2	130	<1.3	<100	11	2,070	3.9	4.8	<15	<1.0	<1.0	0.2
ECRB-SYS-CS1250/5.0-5.7/UC	3	0.2	18	<1.3	<50	22	480	11	22	42	<1.0	<1.0	15
ECRB-SYS-CS1250/3.4-4.0/UC	2.1	M	200	<1.0	50	29	1,390	<8.0	8	150	<1.0	<1.0	3.6
ECRB-SYS-CS800/4.9-5.6/UC	1.6	M	34	<1.0	<25	12	1,140	6.7	6.3	36	<1.0	<1.0	0.9
ECRB-SYS-CS700/5.5-5.8/UC	6.2	<0.1	330	<7.5	<300	22	2,970	<18	18	72	<2.5	<6.0	6.1

Source: DTN: GS020408312272.003 [DIRS 160899].

NOTE: F and Br are in mg/L; all others are mg/L; M indicates not measured.

[1] Greater than 200 ppb tungsten in sample, resulting in possible interference for Hg.

Table 6.5-2. MineralSuppressions that are Used in the Engineered Barrier System Physical and Chemical Environment Geochemical Modeling

Mineral	Formula	Criteria Selected	Rationale	References
Cristobalite (alpha)	SiO ₂	Criterion 2	Cristobalite is thermodynamically stable at temperatures greater than 1,470°C. At standard temperatures and pressures, cristobalite will slowly convert to quartz.	Krauskopf 1979 [DIRS 105909], Figure 14-1, Table 6.4.4-1
Dolomite	CaMg(CO ₃) ₂	Criterion 2	Although dolomite is a common mineral in evaporite deposits from springs derived from carbonate and tuffaceous waters in southern Nevada at Yucca Mountain, its growth mechanism is slow when compared to the precipitation calcite, opal and Mg-bearing minerals, such as sepiolite.	Vaniman et al. 1992 [DIRS 107066], Table 6.4.4-1
Glaserite	NaK ₃ (SO ₄) ₂	Criterion 4	Although glaserite is a mineral that is expected to form in evaporitic type deposits, at the time modeling runs for this document were initiated, the thermodynamic data for glaserite being considered for inclusion in the Pitzer database was in question.	This mineral was suppressed, subject to sensitivity analysis (see Section 6.12.4.4 for results of the sensitivity analysis)
Magnesite	MgCO ₃	Criterion 4	Magnesite is commonly associated with metamorphic mineral assemblages, such as serpentine. There are instances where magnesite is associated with salt deposits, yet it is uncertain that it can form under standard temperatures and pressures as magnesite could be associated with the diagenesis of buried salt deposits.	Kerr 1977 [DIRS 161606] Eugster and Hardie 1978 [DIRS 100743] This mineral would be suppressed, subject to sensitivity analysis (see Section 6.12.4.4 for results of the sensitivity analysis)

Table 6.5-2. MineralSuppressions that are Used in the Engineered Barrier System Physical and Chemical Environment Geochemical Modeling (Continued)

Mineral	Formula	Criteria Selected	Rationale	References
Maximum Microcline	KAlSi_3O_8	Criterion 1	Microcline is generally associated with the formation of granite, syenite, and gneiss. Although it is often found as a common mineral in sandstone or arkose, the occurrence in these instances is detrital.	Kerr 1977 [DIRS 161606], p. 306, Table 6.4.4-1
Quartz	SiO_2	Criterion 2	Literature evidence suggests that amorphous silica is at metastable equilibrium with respect to quartz at low temperatures and pressures. This is also evidenced by the precipitation of opal-A (an amorphous silica phase) as opposed to quartz in evaporated carbonate and tuffaceous waters of southern Nevada.	Langmuir 1997 [DIRS 100051] Vaniman et al. 1992 [DIRS 107066], Table 6.4.4-1
Talc	$\text{Mg}_3\text{Si}_4\text{O}_{10}(\text{OH})_2$	Criterion 1	Talc is characteristically associated with low-grade metamorphic rock and hydrothermal alteration of ultrabasic rocks.	Kerr 1977 [DIRS 161606], Table 6.4.4-1
Ca-saponite Mg-saponite Na-saponite H-saponite K-saponite	$\text{Ca}_{0.165}\text{Mg}_3\text{Al}_{0.33}\text{Si}_{3.67}\text{O}_{10}(\text{OH})_2$ $\text{Mg}_{3.165}\text{Al}_{0.33}\text{Si}_{3.67}\text{O}_{10}(\text{OH})_2$ $\text{Na}_{0.33}\text{Mg}_3\text{Al}_{0.33}\text{Si}_{3.67}\text{O}_{10}(\text{OH})_2$ $\text{H}_{0.33}\text{Mg}_3\text{Al}_{0.33}\text{Si}_{3.67}\text{O}_{10}(\text{OH})_2$ $\text{K}_{0.33}\text{Mg}_3\text{Al}_{0.33}\text{Si}_{3.67}\text{O}_{10}(\text{OH})_2$	Criterion 1	Saponite is a montmorillonite or smectite clay. Smectite clays are commonly associated with fracture linings at Yucca Mountain. However, saponitic clays are associated with the weathering of basalt and not rhyolitic tuffs. Saponite does not generally form independently from its associated parent material, nor does it precipitate independently in soil environments.	Krauskopf 1979 [DIRS 105909] Carlos et al. 1995 [DIRS 105213] Deer et al. 1966 [DIRS 162338] Borchardt 1989 [DIRS 156639]

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

Mineral	Formula	Criteria Selected	Rationale	References
Calcite	CaCO_3	Criterion 3	Calcite is a common evaporite mineral formed from evaporated waters of southern Nevada.	Vaniman et al. 1992 [DIRS 107066]
$\text{SiO}_2(\text{am})$	SiO_2	Criterion 2	Literature evidence suggests that amorphous silica is at metastable equilibrium with respect to quartz at low temperatures and pressures. This is also evidenced by precipitation of opal-A as opposed to quartz in evaporated carbonate and tuffaceous waters of southern Nevada	Langmuir 1997 [DIRS 100051] Vaniman et al. 1992 [DIRS 107066]
Fluorite	CaF_2	Criterion 3	Fluorite is associated with evaporite deposits in Nevada playas.	Papke 1976 [DIRS 162274], Tables 1 and 6.4.4-1
Sepiolite	$\text{Mg}_4\text{Si}_6\text{O}_{15}(\text{OH})_2 \cdot 6\text{H}_2\text{O}$	Criterion 3	The precipitation of sepiolite is common in conjunction with calcite precipitation in calcrete deposits. Sepiolite is a common fracture-lining mineral above the basalt vitrophyre of the Topopah Spring Member at Yucca Mountain. Sepiolite is also known to commonly form on evaporation of either carbonate-source or tuff-source waters in southern Nevada.	Hay and Wiggins 1980 [DIRS 162281] Carlos et al. 1995 [DIRS 105213] Vaniman et al. 1992 [DIRS 107066]
Celadonite	$\text{KMgAlSi}_4\text{O}_{10}(\text{OH})_2$	Criterion 3	Although its occurrence is generally associated with hydrothermally altered mafic volcanic rocks and with illite-chlorite minerals, celadonite is also found as an authigenic silicate mineral in saline, alkaline, and nonmarine environments such as playa deposits.	Li et al. 1997 [DIRS 159034] Hay et al. 1966 [DIRS 105965]
Thenardite	Na_2SO_4	Criterion 3	Thenardite is associated with evaporite deposits in Nevada playas.	Papke 1976 [DIRS 162274], Table 1
Halite	NaCl	Criterion 3	Halite is associated with evaporite deposits in Nevada playas.	Papke 1976 [DIRS 162274], Table 1 Kerr 1979 [DIRS 161606], p. 221, Table 6.4.4-1
Huntite	$\text{CaMg}_3(\text{CO}_3)_4$	Criterion 3	Huntite is a Mg carbonate mineral associated with cave and evaporite deposits as well as with meteoric (low-temperature) dissolution, and re-precipitation of calcite, dolomite, or magnite. Huntite will precipitate instead of calcite when Mg^{2+} is concentrated in solutions with respect to Ca^{2+} due to evaporative processes.	Faust 1953 [DIRS 162282] Walling et al. 1995 [DIRS 162283], p. 360
Sellaite	MgF_2	Criterion 3	Sellaite is the Mg analog to fluorite that forms in evaporite deposits.	Palache et al. 1951 [DIRS 162280], pp. 37 to 39
Gypsum	$\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$	Criterion 3	Gypsum is associated with evaporite deposits in Nevada playas.	Papke 1976 [DIRS 162274], Table 1 Kerr 1979 [DIRS 161606], p. 221, Table 6.4.4-1

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
Glauberite	$\text{Na}_2\text{Ca}(\text{SO}_4)_2$	Criterion 3	Glauberite is associated with evaporite deposits in Nevada playas.	Papke 1976 [DIRS 162274], Table 1
Niter	KNO_3	Criterion 3	Niter is associated with evaporite deposits in Nevada playas.	Papke 1976 [DIRS 162274], Table 1
Sylvite	KCl	Criterion 3	Sylvite is associated with evaporite deposits in Nevada playas.	Papke 1976 [DIRS 162274], Table 1 Kerr 1979 [DIRS 161606], p. 221
Arcanite	K_2SO_4	Criterion 3	Arcanite is a very soluble mineral belonging to the Mascagnite group and can be precipitated in the laboratory from the slow evaporation of water solutions. This mineral is related to thenardite and should have similar properties.	Palache et al. 1951 [DIRS 162280], pp. 398 to 400
Soda Niter	NaNO_3	Criterion 3	Soda Niter is associated with evaporite deposits in Nevada playas.	Papke 1976 [DIRS 162274], Table 1
Carnallite	$\text{KMgCl}_3 \cdot 6\text{H}_2\text{O}$	Criterion 3	Carnallite is associated with evaporite deposits in Nevada playas.	Papke 1976 [DIRS 162274], Table 1 Kerr 1979 [DIRS 161606], p. 221
Pentasalt (Gorgeyite)	$\text{K}_2\text{Ca}_5(\text{SO}_4)_6 \cdot \text{H}_2\text{O}$	Criterion 3	Gorgeyite occurs in association with glauberite, halite, and polyhalite in salt deposits.	Fleischer and Efremov 1954 [DIRS 162312]
Syngenite	$\text{K}_2\text{Ca}(\text{SO}_4)_2 \cdot \text{H}_2\text{O}$	Criterion 3	Syngenite is associated with salt deposits (especially halite) and precipitates in cavities created by volcanic action. It precipitates at room temperatures from solutions that contain K_2SO_4 .	Palache et al. 1951 [DIRS 162280], pp. 442 to 444
Anhydrite	CaSO_4	Criterion 3	Anhydrite is associated with evaporite deposits in Nevada playas.	Papke 1976 [DIRS 162274], Table 1 Kerr 1979 [DIRS 161606], p. 221
Natrite	Na_2CO_3	Criterion 3	Natrite is a highly soluble carbonate mineral associated with shortite, pirssonite, and gaylussite. These three minerals are also associated with the precipitation of trona, calcite, and montmorillonite and are found in clay beds that have deposited in borax lakes.	Fleischer and Pabst 1983 [DIRS 162284] Palache et al. 1951 [DIRS 162280]
Trona	$\text{Na}_3\text{H}(\text{CO}_3)_2 \cdot 2\text{H}_2\text{O}$	Criterion 3	Trona is associated with evaporite deposits in Nevada playas.	Papke 1976 [DIRS 162274], Table 1
Burkeite	$\text{Na}_6\text{CO}_3(\text{SO}_4)_2$	Criterion 3	Burkeite is a saline mineral associated with $\text{Na-CO}_3\text{-SO}_4\text{-Cl}$ brines.	Eugster and Hardie 1978 [DIRS 100743], Table 3

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 169856]), 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 169856], 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 169856], 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 169856], 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

carbonate-rich brine (Eugster and Hardie 1978 [DIRS 100743], p. 244). As evaporation continues, other chemical divides will be encountered, as phases precipitate containing, for example, Na, K, Ca, Mg, Cl, CO₃, SO₄, F, or NO₃. Nitrate is not necessarily conserved in a system that contains organics; however, the results of the in-drift microbial communities model concludes (BSC 2004 [DIRS 169991], Section 7.1), "Because of the oxic environment, denitrification is inhibited. Significant microbial consumption of nitrate will not occur." In the end, the composition of the resulting brine will depend heavily on the original ratios of dissolved components.

As described in Section 4.1.3, each of the five THC model runs produce time histories of changing water compositions for the grid blocks of a numerical grid representing the host rock around the drift. Manipulation of the numerical model output produces time histories at 72 locations and 50 discrete points in time over the 100,000-year modeling period. To capture the more rapid fluctuations at early times, these points in time are roughly log-normally distributed over the time period (i.e., durations between these points increase with time). In total, there are approximately 3,600 discrete water chemistries per THC output. Thus, the inputs listed on Table 4.1-13 contain 18,000 ($5 \times 72 \times 50$) water chemistries. There are then further reductions in this number using the selection process as defined within *Post-Processing Analysis for THC Seepage* (BSC 2004 [DIRS 169858], Section 6.2.3.3) down to 368 water chemistries.

An abstraction method is used to generate lookup tables to represent the effects of evaporation within the drift for any given period. Five steps are required to abstract the THC results using this method. That sequence of steps is repeated for each of the five compositions of percolating water (w0, w4, w5, w6, and w7). The five steps are as follows:

- Step 1: Obtain the THC seepage abstraction model output for the five starting-water compositions (Section 6.6.2).
- Step 2: Use *In-Drift Precipitates/Salts Model* (BSC 2004 [DIRS 169863]) to calculate compositions that result from the seepage waters evaporation identified in Step 1 to a common water activity equal to 0.65. This step characterizes the seepage compositions by chemical properties of the waters they yield when concentrated by evaporation, the in-drift process of concern (Section 6.6.3).
- Step 3: Sort the evaporated seepage water compositions from Step 2 into groups that exhibit similar chemical characteristics, placing into a single bin those seepage water compositions from Step 1. The result is a set of seepage water composition bins, each populated with compositions that yield chemically similar solutions after they are concentrated by evaporation (Section 6.6.4).
- Step 4: Identify the median water composition in each bin and use it as an approximation of all the seepage water compositions within the bin (Section 6.6.5).
- Step 5: Approximate each THC output seepage water composition time history with a time-sequence of median bin compositions derived from Step 4 (Section 6.6.6).

6.6.2 Thermal-Hydrological-Chemical Seepage Abstraction Model Results (Step 1)

The abstracted output of the THC seepage results is presented in *Post-Processing Analysis for THC Seepage* (BSC 2004 [DIRS 169858], Section 6.2.3.3), where water compositions are spatially selected to represent the potential seepage compositions through time. The THC product output files containing the inventory of possible seepage waters are listed in Table 4.1-13. The selection described in *Post-Processing Analysis for THC Seepage* (BSC 2004 [DIRS 169858], Section 6.2.3.3) further reduces this inventory to produce the final set of 368 water compositions that are used as direct input to this model. These water selections are listed in Table 6.6-1.

Table 6.6-1 is a summary of the seepage water inputs. The right-hand column in Table 6.6-1 gives the points in time (which also coincides with the filenames) that were used.

6.6.3 Evaporate Waters to a Common Degree of Concentration (Step 2)

The seepage water compositions from the THC model identified in Step 1 vary over time not only in terms of the molal ratios of the dissolved constituents, but also in terms of the absolute concentrations of these constituents. To group these calculated seepage water compositions into bins containing relatively homogeneous water types, these waters are normalized (based on same activity of water) to reflect the compositions of water by evaporating them to a common activity of water.

The in-drift precipitates/salts model (BSC 2004 [DIRS 169863]) is used to calculate normalized seepage water compositions resulting from evaporation of the more than 300 waters identified in Step 1. This approach accounts for the effects of nearly all chemical divides important to a particular water. Other methods, such as dividing each concentration by the ionic strength, cannot accurately reveal the likely brine endpoint for a given water, which is important to establishing corrosion rates germane to performance assessment. As determined by the in-drift precipitates/salts model evaporations, the waters evaporatively evolve to several different brine types, most commonly nitrate brines, chloride brines, and their combinations. An activity of water of 0.65 was chosen as the common endpoint of these evaporation runs (at equilibrium, the water activity is equivalent to the relative humidity) because this is the lowest approximate value in which all runs are above the deliquescence point.

The EQ3/6 program input files used in the in-drift precipitates/salts model evaporation calculations are generated according to the protocol outlined in *In-Drift Precipitates/Salts Model* (BSC 2004 [DIRS 169863]) using the EQ3/6 program template files found in DTN: MO0303SPAMEQ36.000 [DIRS 162549]. Temperature, pH, carbon dioxide partial pressure, and concentrations of dissolved components tracked in the THC model are taken directly from the THC model output, except for Fe. The predominate iron species (Fe^{3+}) is excluded as it is a relatively insoluble ($< 2 \times 10^{-10}$ molal) species and of no consequence to the evaporated brine composition. Electrical balancing is performed using the aqueous component whose molality (mole/kg solution) would be least affected on a percentage basis. The minerals suppressed in these calculation runs are discussed in Section 6.5.5. In addition to the list of minerals provided on Table 6.5-2, three additional minerals (albite, k-feldspar and celadonite)

that were not originally included in the in-drift precipitates/salts model mineral suppression list, are suppressed in a few of the calculation runs.

Table 6.6-1. Locations and Identification of Seepage Water Compositions to be Binned

Starting Water Composition	Worksheet: Quadrant: Zone: Index:	Case Abbreviation	Points in Time Specific to Case ^A	Points in Time Common to All Cases ^A
HD-PERM water (Alcove 5) <i>thc6_w0_r.xls</i>	"fractures-ch" "Top" "Front" "4"	w0tf4	789, 12,310	10, 51, 53, 55, 60, 75, 100, 150, 200, 250, 300, 350, 400, 500, 600, 650, 700, 750, 800, 1,000, 1,200, 1,400, 1,601, 1,801, 2,001, 2,201, 2,401, 3,002, 5,003, 7,004, 10,006, 15,010, 20,013, 50,034
	"matrix-ch" "Base" "Front" "4"	w0bf4		
Cross-drift water CS2000/16.5 <i>thc6_w4_r.xls</i>	"fractures-ch" "Top" "Front" "4"	W4tf4	804, 2,597, 12,597	
	"matrix-ch" "Base" "Front" "4"	W4bf4		
Cross-drift water CS1000/7.3 <i>thc6_w5_r.xls</i>	"fractures-ch" "Top" "Front" "4"	w5tf4	784, 2,392, 12,304	
	"matrix-ch" "Base" "Front" "4"	w5bf4		
Boreholewater SD-9/990.4 <i>thc6_w6_r.xls</i>	"fractures-ch" "Top" "Front" "4"	w6tf4	865, 3,048, 13,053	
	"matrix-ch" "Base" "Front" "4"	w6bf4		
Cross-drift water CS500/12.0 <i>thc6_w7_r.xls</i>	"fractures-ch" "Top" "Front" "4"	w7tf4	784, 2,591, 12,596	
	"matrix-ch" "Base" "Front" "4"	w7bf4		

Source: Starting water compositions: DTN: LB0302DSCPTHCS.002 [DIRS 161976].

NOTE: EQ3 and EQ6 input and output filenames are the same as the points in time with the extensions: *.3i, 3o, 6i, 6o, respectively, and are archived in output DTN: MO0303MWDEBSSM.000 (EQ3) and output DTN: MO0303MWDEBSSM.000 (EQ6).

^a Some values differ by -1 from the values in source DTN: LB0302DSCPTHCS.002 [DIRS 161976] due to rounding errors.

The rationale for suppression of these three minerals is included on Table 6.6-2. These suppressions are also made in the modeling runs found in Section 6.9. The fugacity of carbon dioxide is set at the volume fraction value provided by the THC model output (Section 6.6.7.2), and that of oxygen is set at the approximate atmospheric value of $10^{-0.7}$ (Table 4.1-16 and Section 6.7). The model runs are set to stop evaporation when the activity of water reaches 0.65 (evaporations start with $a_w \approx 1.0$).

Table 6.6-2. Additional Mineral Suppressions Included During Evaporation to 65 Percent Relative Humidity

Mineral	Formula	Criteria Selected	Rationale	References
Albite	$\text{NaAlSi}_3\text{O}_8$	Criterion 2	Albite is a common mineral in felsic volcanic and plutonic rocks. It can also form in low-grade metamorphic greenschist facies. It forms at normal pressures at temperatures around 700°C. The formation of albite is kinetically retarded at low temperatures.	Frye 1981 [DIRS 161804], p. 538 Deer et al. 1992 [DIRS 163286], p. 401
K-feldspar	KAISi_3O_8	Criterion 2	K-feldspars such as sanidine and microcline are commonly found in plutonic rocks and pegmatites and are found in gneisses. K-feldspars generally form at temperatures between 700°C and 500°C. The formation of K-feldspar is kinetically retarded at diagenetic temperatures ($\leq 200^\circ\text{C}$). The formation of K-feldspar in low temperature metamorphic rocks is common but typically $\geq 200^\circ\text{C}$.	Frye 1981 [DIRS 161804], pp. 669 to 670 Deer et al. 1992 [DIRS 163286], Figure 130
Celadonite	$\text{KMgAlSi}_4\text{O}_{10}(\text{OH})_2$	Criterion 2	Celadonite is a mica mineral similar to glauconite that occurs mostly in basalts. The occurrences are in vesicles or as replacements of ferromagnesian constituents.	Deer et al. 1992 [DIRS 163286], p. 297

Table 6.6-1 lists the input and output files generated for use in EQ3/6 calculations, along with the DTNs in which the files are archived. The filenames correspond to the year for which the water composition prediction is documented by the THC model. With these approximations and the rationale for abstraction, the number of input waters is reduced from 18,000 to 368. The full set of input and output files generated is included in output DTNs: MO0303MWDSCMAB.000 and MO0303MWDEBSSM.000.

6.6.4 Seepage Water Composition Bin Generation (Step 3)

The final equilibration results from each output file as listed on Table 6.6-1 and archived in output DTN: MO0303MWDEBSSM.000, are tabulated using the GETEQDATA software to create *Final Checked EBS Seepage Binning Abstraction Rev 4.xls*. This spreadsheet is archived in DTN: MO0310SPAEBSCB.003 and contains the output variables: pH, activity of water ($a_w \approx 0.65$), ionic strength (I), total molalities of the aqueous constituents, and cumulative log moles of minerals precipitated. In addition, formulas are added to calculate various molar ratios and the hydrogen ion activity, and several graphs are inserted to illustrate the variability in the outputs and calculations (Figures 6.6-5 to 6.6-7). These graphs are ordered primarily by the five

different starting waters, and then each of those outputs ordered by time. This information is needed before the waters can be grouped by similarity.

(Figures 6.6-1 through 6.6.4 intentionally deleted.)

Source: Output DTN: MO0310SPAEBSCB.003.

Figure 6.6-5. Selected Molal Ratios (Cl/N, Cl/S, Cl/Na, Cl/F, Na/K, Cl/C, K/N, and Na/C) from the Evaporation of the 368 Seepage Waters to 65 Percent Relative Humidity, Used in the Binning Analysis to Establish Binning Criteria

Source: Output DTN: MO0310SPAEBSCB.003.

Figure 6.6-6. Selected Molal Ratios (Cl/N, Cl/S, Cl/Na, Ca/K, Ca/C, Cl/C and Ca/N) from the Evaporation of the 368 Seepage Waters to 65 Percent Relative Humidity, Used in the Binning Analysis to Establish Binning Criteria

Source: Output DTN: MO0310SPAEB5CB.003.

Figure 6.6-7. Mineral Assemblages of the 368 Selected Seepage Waters After Evaporation to 65 Percent Relative Humidity

Binning of the seepage water compositions identified in Step 1 is accomplished by group sorting, such that all the seepage waters in a group yield chemically similar solution compositions after they are concentrated by evaporation. Eight characteristic properties are identified for determining that chemical similarity. They are defined in such a way that they yield low intrabin composition ranges compared with the composition ranges existing among all of the waters.

The evaporated waters are binned based on the following eight criteria:

- Total aqueous Ca molality > 0.01 molal?
  - If yes, the water likely evaporatively evolves on the calcium side of the calcite and gypsum chemical divides, resulting in brine that is depleted of carbonate and sulfate. These brines also tend to have neutral to acidic pH.
- Total aqueous CO_3 molality < 0.1 molal?
  - If no, Ca is likely depleted by the precipitation of calcite. In some cases, Ca and CO_3 have low concentrations, so this criterion further divides brines with Ca molality less than 0.1 molal. Waters having low concentrations of both of these components tend to maintain a neutral pH as they evaporate.
- Total aqueous Ca molality > total aqueous Na molality?
  - This criterion segregates bin 1 and bin 2 waters.
- Total aqueous Ca molality > total aqueous K molality?
  - This criterion segregates bin 2 and bin 3 waters. Without this criterion, K and Ca would have large variability ranges in a combined 2+3 bin.

- Total aqueous NO_3 molality > total aqueous CO_3 molality?
  - This criterion segregates bin 9 and bin 11 waters. Without this criterion, a combined 9+11 bin would have larger variations within the bin, especially for NO_3 .
- Total aqueous F molality < 0.1 molal?
  - This criterion distinguishes waters in bin 6 from bin 9 and waters in bin 8 from bin 10. Without this criterion, combined 6+9 and 8+10 bins would have larger variabilities within the bins.
- Total aqueous F molality < 0.03 molal?
  - This criterion distinguishes waters in bin 7 from bin 8. Without this criterion, a combined 7+8 bin would have much larger variability within the bin for many of the components.
- Total aqueous SO_4 molality > 1 molal?
  - This criterion distinguishes waters in bin 6 from bin 8 and waters in bin 9 from bin 10. Without this criterion, combined 6+8 and 9+10 bins would have larger variabilities within the bins for many output parameters.

Columns containing “if/then/else” formulas are added to the spreadsheet to facilitate responding to each criterion for each water. Waters having identical answers to the questions listed on Table 6.6-3 are placed in the same bin. Eleven bins are similarly defined.

Table 6.6-3. Binning Criteria Answer Key

Bin	$\text{Ca} > 0.01\text{m}$	$\text{Ca} > \text{Na}$	$\text{CO}_3 < 0.1\text{m}$	$\text{Ca} > \text{K}$	$\text{NO}_3 > \text{CO}_3$	$\text{F} < 0.1\text{m}$	$\text{F} < 0.03\text{m}$	$\text{SO}_4 > 1\text{m}$
1	yes	yes	yes	yes	yes	yes	yes	no
2	yes	no	yes	yes	yes	yes	yes	no
3	yes	no	yes	no	yes	yes	yes	no
4	no	no	yes	no	yes	yes	yes	no
5	no	no	yes	no	yes	yes	yes	yes
6	no	no	no	no	yes	yes	no	no
7	no	no	no	no	yes	yes	yes	yes
8	no	no	no	no	yes	yes	no	yes
9	no	no	no	no	yes	no	no	no
10	no	no	no	no	yes	no	no	yes
11	no	no	no	no	no	no	no	no

Source: Output DTN: MO0310SPAEBSCB.003.

Results are provided in *Final Checked EBS Seepage Binning Abstraction Rev 4.xls* (DTN: MO0310SPAEBSCB.003). These are also shown in Figure 6.6-8 for all water compositions, as sequentially sorted into bins 1 through 11, and shows visually distinct groupings of the compositions contained within each of the eleven bins. Figures 6.6-9 through 6.6-19 show the water compositions for each bin separately. A comparison of these

plots with the previous plots showing all of the evaporated water compositions before binning (Figures 6.6-5 to 6.6-7) illustrates that the binning process is successful in grouping waters with similar compositions in the same bin. The pH results are especially salient, as it is not an explicit binning criterion. The pH covers a wide range in the initial waters, and is well segregated into the resulting bins as shown in Figure 6.6-8.

Source: Output DTN: MO0310SPAEBSCB.003.

Figure 6.6-8. Evaporated Water Compositions for All Bins Sorted by Bin After Evaporation to 65 Percent Relative Humidity

Source: Output DTN: MO0310SPAEBSCB.003.

Figure 6.6-9. Evaporated Water Compositions for Bin 1 After Evaporation to 65 Percent Relative Humidity

Source: Output DTN: MO0310SPAEBSCB.003.

Figure 6.6-10. Evaporated Water Compositions for Bin 2 After Evaporation to 65 Percent Relative Humidity

Source: Output DTN: MO0310SPAEBSCB.003.

Figure 6.6-11. Evaporated Water Compositions for Bin 3 After Evaporation to 65 Percent Relative Humidity

Source: Output DTN: MO0310SPAEBSCB.003.

Figure 6.6-12. Evaporated Water Compositions for Bin 4 After Evaporation to 65 Percent Relative Humidity

Source: Output DTN: MO0310SPAEBSCB.003.

Figure 6.6-13. Evaporated Water Compositions for Bin 5 After Evaporation to 65 Percent Relative Humidity

Source: Output DTN: MO0310SPAEBSCB.003.

Figure 6.6-14. Evaporated Water Compositions for Bin 6 After Evaporation to 65 Percent Relative Humidity

Source: Output DTN: MO0310SPAEBSCB.003.

Figure 6.6-15. Evaporated Water Compositions for Bin 7 After Evaporation to 65 Percent Relative Humidity

Source: Output DTN: MO0310SPAEBSCB.003.

Figure 6.6-16. Evaporated Water Compositions for Bin 8 After Evaporation to 65 Percent Relative Humidity

Source: Output DTN: MO0310SPAEBSCB.003.

Figure 6.6-17. Evaporated Water Compositions for Bin 9 After Evaporation to 65 Percent Relative Humidity

Source: Output DTN: MO0310SPAEBSCB.003.

Figure 6.6-18. Evaporated Water Compositions for Bin 10 After Evaporation to 65 Percent Relative Humidity

Source: Output DTN: MO0310SPAEBSCB.003.

Figure 6.6-19. Evaporated Water Compositions for Bin 11 After Evaporation to 65 Percent Relative Humidity

Binning Efficacy—The effectiveness of the binning process is measured by how well it reduces the variability of important chemical parameters. Table 6.6-3A demonstrates that the binning procedure was effective in segregating the water chemistries. For example, the overall standard deviation in pH of all 65 percent relative humidity waters is 1.12, while the average of the standard deviations of those waters in their eleven bins is 0.20 (nearly a factor of 6 decrease in the standard deviation). Binning is also very effective for calcium (reduced deviation by factor of 7), and somewhat effective for segregating chloride and nitrate (near a factor of 2 reduction in deviation).

Table 6.6-3a. Standard Deviation of In-Drift Water Chemistry at 65 percent Relative Humidity, Before and After Binning

	Waters (n)	Standard Deviation of pH	Standard Deviation of Ca (mol/kg. H ₂ O)	Standard Deviation of Cl (mol/kg. H ₂ O)	Standard Deviation of NO ₃ (mol/kg. H ₂ O)
Bin 1	5	0.08	0.29	0.92	1.05
Bin 2	13	0.11	0.28	0.68	0.83
Bin 3	12	0.24	0.42	0.4	0.56
Bin 4	43	0.34	<0.01	1.87	2.79
Bin 5	27	0.29	<0.01	0.32	0.56
Bin 6	8	0.37	<0.01	1.65	2.73
Bin 7	25	0.16	<0.01	0.5	0.81
Bin 8	22	0.14	<0.01	0.73	1.43
Bin 9	58	0.22	<0.01	0.61	0.91
Bin 10	10	0.1	<0.01	0.5	0.85
Bin 11	145	0.19	<0.01	0.39	0.15
Average Bins 1 to 11 ^a		0.2	0.09	0.78	1.15
All Waters, no binning		1.12	0.63	1.21	1.94

A second binning approach that uses characteristic properties of precipitating mineral assemblages to sort and generate the bins has also been evaluated. This approach is considered an alternate conceptual model and is documented in Section 6.11.

6.6.5 Choice of Representative Seepage Water for Each Bin (Step 4)

A median seepage water composition for each bin is chosen to represent all seepage water compositions in that bin. Table 6.6-4 provides the median water identifiers for each of the eleven bins defined in Section 6.6.4, and Table 6.6-5 provides the median seepage water compositions for each bin. A description of the method for that process is described as follows. All 368 unevaporated seepage water compositions corresponding to the evaporated waters binned in Step 3 are sorted by bin and copied into separate bin worksheets (e.g., Bin 11 abstract, Bin 10 abstract). This information is found in the data and plots worksheet in *Final Checked EBS Seepage Binning Abstraction Rev 4.xls* (DTN: MO0310SPAEBSCB.003). These worksheets are used to determine a representative median water for each bin, as well as individual bin statistics. In so doing, the abstraction further reduces from 368 to 11 the set of representative seepage waters. These 11 water compositions are then used as inputs into the model calculations performed in Section 6.9.

Table 6.6-4. Median Water Identifier for Each Bin and Percentage in Each Bin

Abstracted Water Compositions			Number of Waters In the Bin	% of All Evaporated Waters Represented by the Bin
Case	Water	Filename		
Bin 1	w7bf4	75.6o	5	1.36
Bin 2	w0bf4	250.6o	13	3.53
Bin 3	w0bf4	650.6o	12	3.26
Bin 4	w4bft	600.6o	43	11.68
Bin 5	w7tf4	300.6o	27	7.34
Bin 6	w0tf4	7004.6o	8	2.17
Bin 7	w4bf4	10006.6o	25	6.79
Bin 8	w5tf4	20013.6o	22	5.98
Bin 9	w6tf4	51.6o	58	15.76
Bin 10	w5bf4	10006.6o	10	2.72
Bin 11	w4tf4	300.6o	145	39.40

Source: Output DTN: MO0310SPAEBSCB.003.

The selected bin chemistry is as close to the median chemistry within the bin as can be obtained without actually using the individual median, minimum, and maximum values calculated in each bin for each independent aqueous species. This approach is designed to maintain consistency with the evaporated EQ6 results, because the starting water used in the EQ3/6 evaluation is a specific time-dependent result from the THC model. In addition, this approach maintains charge balance (sum of cations versus anions), which is important in evaporation calculations.

Median Water—A methodology is used to determine the median water from each of the 11 bins. Internal Excel functions are used to determine the statistical rank (1 through 12) for each set of twelve parameters (i.e., pH, Al, C, Ca, Cl, F, K, Mg, N, Na, S, and Si) among all the waters in one individual bin. A median water is selected by determining which waters contain the median value for each parameter, and then using the COUNTIF function, and summing the number of these median value parameters captured by each water in that bin. If two waters of a single bin contain equivalent numbers of median value parameters, then the number of “near median” values (parameter values on either side of the median) are next considered, with the water containing the greatest number of these then being designated as the median water to represent that bin. Table 6.6-4 lists the water selection results of the median water for each bin.

In addition, the distribution of all waters is calculated among the bins by counting the total number of waters contained within each bin and determining the percentage of waters represented in each bin; these results are also shown on Table 6.6-4. Bin 11 contains the largest number of waters and thus is the most likely median water. Bins 11, 4, and 9 make up the composition of over 66 percent of all of the waters. Each of the EQ6 filenames listed on Table 6.6-4 were mapped back to the values found on the THC spreadsheets listed on Table 6.6-1 to create Table 6.6-5 which contains the 11 complete starting water compositions and associated partial pressures of carbon dioxide.

Within each of the 11 “bin abstract” worksheets, the median, minimum, maximum standard deviation(s), and two standard deviations (2s) are calculated. Table 6.6-6 contains the individual parameter statistics for each bin, which, when compared to similar statistics for data shown on

the data and plots worksheet, indicate that the within bin statistics are generally much smaller than the entire group of data (Table 6.6-7).

6.6.6 Abstraction of THC Model Outputs - Defining Time Sequences of Bins that Approximate Seepage Water Composition Time Histories from THC Model Outputs (Step 5)

In this section, each THC model realization (time history of seepage water compositions) is abstracted in the form of a time-sequence of the seepage water bin median compositions. For simplicity, the term "bin," henceforth, refers to the median composition for a bin, as well as to its contents, and the term "bin map" refers to time sequences of seepage water bin median compositions abstracted from a THC model realization.

The bin maps for THC outputs are generated using the bin definitions given in Section 6.6.4 and the THC output time defined in Section 6.6.2 (Step 1). The following bin-mapping process was applied to each of the ten combinations of water composition parameter (QUADR, ZONE, and INDEX) values, and worksheets (fractures-ch and matrix-ch) from THC model outputs (defined in Section 6.6.2, Step 1, summarized in Table 6.6-1):

1. Define a time interval around each of the THC output time values that are identified in Step 1 of the binning process (Section 6.6.2 and fourth and fifth columns of Table 6.6-1) for each of the combinations described above (e.g., the combination for case w0tf4). Begin and end the time intervals approximately midway between adjacent time values. For example, in Table 6.6-8 (applicable to water w0) for the THC output time value of 800 years (in EQ6 Output Filename 800.60), the time interval begins at 794.5 years (between 789 and 800 years) and ends at 900 years (between 800 and 1,000 years).
2. Assign to that time interval the bin (bin median composition) that contains the seepage water composition from the THC output at the output time around which the time interval was defined. For example, in Table 6.6-8, bin 11 is assigned to time interval 794.5 to 900 years for crown seepage (Quadrant = Top), because the THC seepage water output composition for case w0tf4 at 800 years (EQ6 Output Filename 800.6) is placed into bin 11 during the binning process.
3. Sequentially repeat items 1 and 2, directly above, for each THC output time.

Table 6.6-5. Initial Compositions of the 11 Binned THC Seepage Waters

Species	Bin 1	Bin 2	Bin 3	Bin 4	Bin 5	Bin 6	Bin 7	Bin 8	Bin 9	Bin 10	Bin 11
Water/ File Name	w7bf4 / 75.60	w0bf4 / 250.60	w0bf4 / 650.60	w4bf4 / 600.60	w7tf4 / 300.60	w0tf4 / 7004.60	w4bf4 / 10006.60	w5tf4 / 20013.60	w6tf4 / 51.60	w5bf4 / 10006.60	w4tf4 / 300.60
T (°C)	111.9	109.1	104.3	104.9	95.62	65.13	56.34	40.18	91.78	56.34	95.61
pH	7.407	7.583	7.615	7.896	7.634	7.695	7.768	7.94	8.139	7.815	7.759
Ca ²⁺	1.75E-02	6.49E-03	2.14E-03	1.08E-03	1.36E-03	4.20E-04	4.46E-04	5.73E-04	7.24E-05	3.52E-04	3.34E-04
Mg ²⁺	1.70E-05	2.95E-06	4.13E-06	5.75E-07	1.13E-05	4.82E-05	5.52E-05	8.51E-05	2.54E-07	4.31E-05	6.34E-06
Na ⁺	3.89E-03	2.63E-03	2.67E-03	1.26E-03	5.53E-03	8.09E-03	7.65E-03	7.31E-03	4.27E-03	6.82E-03	4.80E-03
Cl ⁻	2.01E-02	5.02E-03	3.35E-03	1.03E-03	3.28E-03	3.32E-03	7.44E-04	5.61E-04	7.34E-04	6.00E-04	1.30E-03
SiO _{2(aq)}	9.42E-03	7.42E-03	6.96E-03	7.38E-03	1.22E-02	2.90E-03	2.46E-03	1.79E-03	4.15E-03	2.47E-03	1.19E-02
HCO ₃ ⁻	5.57E-05	9.06E-05	1.95E-04	1.64E-04	4.18E-04	2.93E-03	6.72E-03	6.92E-03	2.04E-03	5.74E-03	1.13E-03
SO ₄ ⁻²	8.87E-03	4.89E-03	1.50E-03	5.88E-04	1.77E-03	1.21E-03	4.12E-04	3.55E-04	1.18E-04	3.80E-04	7.29E-04
K ⁺	8.68E-04	5.40E-04	5.00E-04	2.38E-04	8.68E-04	6.25E-04	4.67E-04	2.76E-04	5.02E-04	4.17E-04	7.50E-04
AlO ₂ ⁻	3.27E-08	7.08E-08	5.02E-08	9.97E-08	8.03E-10	5.36E-09	3.62E-09	1.50E-09	6.09E-08	4.03E-09	1.42E-09
F ⁻	1.93E-04	2.46E-04	3.48E-04	4.28E-04	1.00E-03	8.26E-04	7.81E-04	6.43E-04	9.77E-04	8.61E-04	1.38E-03
NO ₃ ⁻	1.30E-03	5.46E-04	1.83E-04	1.33E-04	2.22E-04	1.04E-04	6.87E-05	3.97E-05	3.10E-04	4.25E-05	1.26E-04
CO _{2(g)} (bars)	3.89E-04	4.93E-04	1.04E-03	4.88E-04	1.88E-03	7.06E-03	1.19E-02	6.34E-03	2.94E-03	9.19E-03	4.06E-03
log CO _{2(g)}	-3.410	-3.307	-2.984	-3.312	-2.726	-2.151	-1.926	-2.198	-2.532	-2.037	-2.392

Source: Output DTN: MO0310SPAEBSCB.003.

NOTE: Unless otherwise marked, units are in moles/kg × H₂O.

Each combination is given a case abbreviation in the third column of Table 6.6-1. The first, second, and last periods for each case are special cases. The bin assigned to the 10-year output represents the period from 0 to 50 years. The 51-year output is binned for the period from 50 to 52 years. Lastly, the 50,034-year output is binned for the period from 35,023.5 to 100,000 years.

Tables 6.6-8 through 6.6-12 provide the maps for each seepage water in the binning analysis. The graphic plots of Figures 6.6-20 through 6.6-29 compare the binning assignments to the evaporated THC outputs. These figures graphically illustrate that the bins cover the changes in chemistry at 65 percent relative humidity through time. For example, peaks and valleys in the chemistry output correspond to a visible change in assigned bins.

Source: Output DTN: MO0310SPAEBSCB.003.

Figure 6.6-20. Bins for Evaporated Crown Seepage: Case w0lf4

Source: DTN: Output MO0310SPAEBSCB.003.

Figure 6.6-21. Bins for Evaporated Invert Seepage: Case w0bf4

Source: Output DTN: MO0310SPAEBSCB.003.

Figure 6.6-22. Bins for Evaporated Crown Seepage: Case w4tf4

Source: Output DTN: MO0310SPAEBSCB.003.

Figure 6.6-23. Bins for Evaporated Invert Seepage: Case w4bf4

Source: Output DTN: MO0310SPAEBSCB.003.

Figure 6.6-24. Bins for Evaporated Crown Seepage: Case w5tf4

Source: Output DTN: MO0310SPAEBSCB.003.

Figure 6.6-25. Bins for Evaporated Invert Seepage: Case w5bf4

Source: Output DTN: MO0310SPAEBSCB.003.

Figure 6.6-26. Bins for Evaporated Invert Seepage: Case w6tf4

Source: Output DTN: MO0310SPAEBSCB.003.

Figure 6.6-27. Bins for Evaporated Invert Seepage: Case w6bf4

Source: Output DTN: MO0310SPAEBSCB.003.

Figure 6.6-28. Bins for Evaporated Invert Seepage: Case w7tf4

Source: Output DTN: MO0310SPAEBSCB.003.

Figure 6.6-29. Bins for Evaporated Invert Seepage: Case w7bf4

Table 6.6-6. Calculated Statistics for All Values Within Each Bin (aw = 0.65)

Bin	Statistic	pH	I	Al	C	Ca	Cl	F	K	Mg	N	Na	S	Si	Cl:NO ₃
1	Median	5.59	1.28E+01	3.20E-12	5.54E-04	3.58E+00	8.43E+00	6.31E-05	3.64E-01	9.16E-04	5.45E-01	1.63E+00	1.84E-03	1.48E-03	1.55E+01
	Min	5.53	1.23E+01	3.03E-12	4.03E-04	3.32E+00	6.52E+00	5.92E-05	1.76E-01	4.14E-04	2.73E-01	7.83E-01	1.82E-03	1.22E-03	2.37E+00
	Max	5.72	1.30E+01	3.60E-12	6.19E-04	4.01E+00	8.71E+00	6.99E-05	4.25E-01	1.27E-03	2.75E+00	1.92E+00	2.12E-03	1.61E-03	3.18E+01
	s	0.08	2.96E-01	2.22E-13	8.67E-05	2.88E-01	9.19E-01	4.18E-06	1.13E-01	3.55E-04	1.05E+00	5.00E-01	1.27E-04	1.86E-04	1.26E+01
	2s	0.15	5.93E-01	4.44E-13	1.73E-04	5.76E-01	1.84E+00	8.37E-06	2.25E-01	7.11E-04	2.11E+00	1.00E+00	2.55E-04	3.72E-04	2.53E+01
2	Median	5.69	1.15E+01	2.32E-12	5.74E-04	2.38E+00	8.30E+00	5.20E-05	9.28E-01	1.32E-03	7.62E-01	3.41E+00	1.93E-03	2.20E-03	1.09E+01
	Min	5.46	1.11E+01	1.33E-12	4.32E-04	1.86E+00	6.54E+00	4.41E-05	5.74E-01	4.66E-04	2.84E-01	2.82E+00	1.58E-03	1.90E-03	2.36E+00
	Max	5.79	1.17E+01	3.76E-12	8.94E-04	2.75E+00	8.83E+00	5.51E-05	1.58E+00	2.49E-03	2.83E+00	3.98E+00	2.03E-03	3.00E-03	3.11E+01
	s	0.11	1.98E-01	7.15E-13	1.52E-04	2.75E-01	6.77E-01	3.50E-06	3.32E-01	5.87E-04	8.35E-01	4.13E-01	1.29E-04	3.16E-04	7.74E+00
	2s	0.22	3.97E-01	1.43E-12	3.03E-04	5.51E-01	1.35E+00	6.99E-06	6.64E-01	1.17E-03	1.67E+00	8.27E-01	2.58E-04	6.31E-04	1.55E+01
3	Median	5.88	1.08E+01	1.09E-12	4.55E-04	1.10E+00	8.42E+00	3.79E-05	3.00E+00	1.26E-03	1.02E+00	4.24E+00	2.07E-03	2.29E-03	8.38E+00
	Min	5.62	1.03E+01	9.46E-14	1.56E-04	7.49E-02	7.74E+00	3.56E-05	1.93E+00	1.11E-04	7.05E-01	3.73E+00	1.54E-03	1.74E-03	3.43E+00
	Max	6.55	1.10E+01	3.54E-12	8.21E-04	1.74E+00	8.95E+00	8.47E-05	5.55E+00	2.50E-03	2.26E+00	4.76E+00	8.07E-03	3.27E-03	1.20E+01
	s	0.24	2.18E-01	9.64E-13	1.84E-04	4.24E-01	4.04E-01	1.36E-05	9.15E-01	7.39E-04	5.58E-01	3.22E-01	1.76E-03	5.22E-04	3.16E+00
	2s	0.49	4.35E-01	1.93E-12	3.67E-04	8.48E-01	8.08E-01	2.72E-05	1.83E+00	1.48E-03	1.12E+00	6.45E-01	3.52E-03	1.04E-03	6.33E+00
4	Median	7.13	1.17E+01	2.23E-13	4.23E-04	2.66E-03	7.17E+00	7.53E-04	5.64E+00	2.32E-06	3.64E+00	5.57E+00	3.76E-01	3.45E-03	1.97E+00
	Min	5.94	1.11E+01	4.07E-15	2.13E-04	9.33E-04	2.81E+00	3.28E-04	2.46E+00	2.20E-07	1.73E+00	5.07E+00	1.97E-01	8.22E-04	2.93E-01
	Max	7.62	1.41E+01	1.14E-12	2.10E-03	4.09E-03	8.28E+00	1.91E-03	6.17E+00	3.89E-04	9.90E+00	1.05E+01	8.61E-01	7.35E-03	4.79E+00
	s	0.34	1.02E+00	2.78E-13	3.15E-04	6.45E-04	1.87E+00	2.50E-04	9.45E-01	8.23E-05	2.79E+00	1.69E+00	9.58E-02	1.26E-03	1.41E+00
	2s	0.68	2.04E+00	5.56E-13	6.30E-04	1.29E-03	3.74E+00	5.00E-04	1.89E+00	1.65E-04	5.59E+00	3.38E+00	1.92E-01	2.51E-03	2.83E+00
5	Median	7.6	1.20E+01	1.26E-13	1.53E-03	8.57E-04	7.71E+00	2.29E-03	4.67E+00	9.30E-07	1.20E+00	6.22E+00	1.02E+00	5.51E-03	6.36E+00
	Min	7.26	1.17E+01	5.79E-14	7.97E-04	2.00E-05	6.98E+00	1.98E-03	4.60E+00	3.63E-08	6.30E-01	5.93E+00	1.00E+00	3.15E-03	2.84E+00
	Max	8.64	1.25E+01	3.44E-13	3.19E-02	9.78E-04	8.04E+00	1.91E-02	4.92E+00	7.68E-06	2.46E+00	6.77E+00	1.13E+00	2.45E-02	1.28E+01
	s	0.29	2.49E-01	8.09E-14	5.84E-03	1.72E-04	3.23E-01	3.24E-03	6.75E-02	2.37E-06	5.63E-01	2.39E-01	2.83E-02	3.95E-03	3.34E+00
	2s	0.58	4.97E-01	1.62E-13	1.17E-02	3.44E-04	6.46E-01	6.48E-03	1.35E-01	4.75E-06	1.13E+00	4.77E-01	5.66E-02	7.91E-03	6.68E+00
6	Median	9.01	1.24E+01	1.18E-13	5.03E-01	8.47E-06	6.36E+00	8.67E-02	4.30E+00	6.72E-08	1.45E+00	6.63E+00	8.53E-01	4.45E-02	4.37E+00
	Min	8.37	1.18E+01	1.13E-14	1.64E-01	7.54E-06	3.17E+00	4.91E-02	2.51E+00	2.59E-09	5.55E-01	6.28E+00	7.99E-01	2.03E-02	4.26E-01
	Max	9.68	1.40E+01	2.37E-13	7.96E-01	9.05E-06	7.79E+00	9.15E-02	4.49E+00	4.35E-07	7.43E+00	1.04E+01	9.30E-01	2.46E-01	1.34E+01
	s	0.37	8.46E-01	9.15E-14	2.52E-01	5.58E-07	1.65E+00	1.63E-02	6.66E-01	1.91E-07	2.73E+00	1.52E+00	4.38E-02	7.78E-02	4.87E+00
	2s	0.73	1.69E+00	1.83E-13	5.04E-01	1.12E-06	3.29E+00	3.26E-02	1.33E+00	3.83E-07	5.46E+00	3.04E+00	8.75E-02	1.56E-01	9.75E+00
7	Median	8.73	1.32E+01	3.94E-15	3.51E-01	1.00E-05	5.83E+00	4.42E-02	4.90E+00	1.30E-06	2.81E+00	6.81E+00	1.24E+00	8.04E-03	2.08E+00
	Min	8.52	1.28E+01	2.71E-15	2.57E-01	8.59E-06	4.08E+00	3.12E-02	4.15E+00	3.64E-07	2.33E+00	6.59E+00	1.03E+00	5.57E-03	7.31E-01
	Max	9.13	1.42E+01	5.87E-15	6.49E-01	1.11E-05	7.08E-02	7.08E-02	5.06E+00	2.31E-06	5.59E+00	8.59E+00	1.41E+00	2.00E-02	2.60E+00
	s	0.16	3.72E-01	1.08E-15	1.06E-01	7.70E-07	5.03E-01	1.15E-02	2.40E-01	5.78E-07	8.14E-01	4.96E-01	1.17E-01	4.00E-03	4.80E-01
	2s	0.32	7.44E-01	2.15E-15	2.11E-01	1.54E-06	1.01E+00	2.30E-02	4.81E-01	1.16E-06	1.63E+00	9.93E-01	2.34E-01	7.99E-03	9.60E-01

Table 6.6-6. Calculated Statistics for All Values Within Each Bin (aw = 0.65) (Continued)

Bin	Statistic	pH	I	Al	C	Ca	Cl	F	K	Mg	N	Na	S	Si	Cl:NO ₃
8	Median	8.58	1.43E+01	1.65E-15	2.08E-01	1.14E-05	4.57E+00	2.30E-02	4.63E+00	2.54E-06	3.86E-06	8.05E+00	1.64E+00	4.15E-03	1.19E+00
	Min	8.4	1.36E+01	6.86E-16	1.42E-01	9.56E-06	2.80E+00	1.36E-02	2.93E+00	1.08E-06	3.27E-06	6.99E+00	1.01E+00	2.10E-03	3.30E-01
	Max	8.98	1.49E+01	2.77E-15	2.65E-01	1.51E-05	5.59E+00	2.97E-02	5.23E+00	6.09E-06	8.48E-06	1.07E+01	1.87E+00	6.14E-03	1.71E+00
	s	0.14	3.07E-01	6.66E-16	3.28E-02	1.38E-06	7.31E-01	4.79E-03	6.63E-01	1.21E-06	1.43E-06	9.77E-01	2.38E-01	1.18E-03	3.52E-01
	2s	0.28	6.15E-01	1.33E-15	6.57E-02	2.75E-06	1.46E+00	9.57E-03	1.33E+00	2.43E-06	2.86E-06	1.95E+00	4.76E-01	2.36E-03	7.04E-01
9	Median	9.15	1.35E+01	1.22E-13	1.14E+00	2.57E-06	5.37E+00	2.39E-01	3.93E+00	3.28E-08	2.34E+00	7.51E+00	7.31E-01	9.34E-02	2.36E+00
	Min	8.78	1.23E+01	1.13E-14	5.95E-01	1.00E-06	3.83E+00	1.17E-01	2.75E+00	1.16E-09	8.18E-09	6.41E+00	6.03E-01	1.51E-02	7.51E-01
	Max	9.66	1.48E+01	1.16E-10	1.55E+00	7.53E-06	6.97E+00	2.64E-01	6.25E+00	5.48E-07	5.12E+00	9.58E+00	9.19E-01	3.01E-01	8.53E+00
	s	0.22	5.91E-01	1.52E-11	2.12E-01	1.98E-06	6.09E-01	4.11E-02	8.45E-01	1.65E-07	9.15E-07	9.65E-01	1.07E-01	7.03E-02	1.24E+00
	2s	0.43	1.18E+00	3.05E-11	4.24E-01	3.96E-06	1.22E+00	8.23E-02	1.69E+00	3.29E-07	1.83E+00	1.93E+00	2.14E-01	1.41E-01	2.49E+00
10	Median	8.75	1.32E+01	1.04E-14	4.12E-01	5.64E-07	5.33E+00	2.07E-01	4.60E+00	4.08E-07	3.37E+00	7.32E+00	1.09E+00	1.02E-02	1.58E+00
	Min	8.7	1.26E+01	4.28E-15	3.02E-01	3.39E-07	4.82E+00	2.05E-01	4.52E+00	3.32E-07	2.21E+00	6.70E+00	1.08E+00	7.76E-03	1.13E+00
	Max	8.97	1.38E+01	1.49E-14	5.06E-01	7.29E-07	6.08E+00	2.12E-01	4.67E+00	5.63E-07	4.25E+00	7.80E+00	1.32E+00	1.43E-02	2.74E+00
	s	0.1	4.62E-01	3.33E-15	7.77E-02	1.55E-07	4.98E-01	2.71E-03	4.66E-02	8.62E-08	8.54E-01	4.34E-01	1.02E-01	2.49E-03	6.78E-01
	2s	0.2	9.24E-01	6.66E-15	1.55E-01	3.10E-07	9.96E-01	5.42E-03	9.33E-02	1.72E-07	1.71E+00	8.67E-01	2.04E-01	4.98E-03	1.36E+00
11	Median	9.17	1.26E+01	1.04E-13	1.16E+00	2.65E-06	6.58E+00	2.42E-01	3.84E+00	3.91E-08	5.58E-01	7.06E+00	6.51E-01	8.12E-02	1.19E+01
	Min	8.85	1.21E+01	2.05E-14	7.35E-01	1.92E-06	3.56E+00	1.04E-01	2.96E+00	3.39E-09	3.27E-01	6.57E+00	6.06E-01	2.46E-02	5.55E+00
	Max	9.72	1.37E+01	2.46E-13	2.06E+00	7.85E-06	7.22E+00	3.34E-01	4.94E+00	3.82E-07	1.14E+00	7.84E+00	9.06E-01	2.98E-01	2.02E+01
	s	0.19	3.22E-01	4.21E-14	1.35E-01	1.81E-06	3.93E-01	4.22E-02	3.30E-01	8.18E-08	1.52E-08	2.61E-01	7.68E-02	5.56E-02	2.82E+00
	2s	0.38	6.44E-01	8.42E-14	2.70E-01	3.63E-06	7.86E-01	8.44E-02	6.60E-01	1.64E-07	3.04E-07	5.23E-01	1.54E-01	1.11E-01	5.63E+00

Source: Output DTN: MO0310SPAEBSCB.003.

NOTE: All units, except pH and Cl:NO₃, are in moles/kg × H₂O.

Table 6.6-7. Calculated Statistics for All Values on the Data and Plots Worksheet

Statistic	pH	I	Al	C	Ca	Cl	F	K	Mg	N	Na	S	Si	Cl:NO ₃
Median	8.98	1.27E+01	1.08E-13	1.04E+00	6.93E-06	6.53E+00	1.48E-01	4.29E+00	2.04E-07	1.25E+00	6.93E+00	6.96E-01	3.79E-02	5.66E+00
Min	5.46	1.03E+01	6.86E-16	1.56E-04	3.39E-07	2.80E+00	3.56E-05	1.76E-01	1.16E-09	2.73E-01	7.83E-01	1.54E-03	8.22E-04	2.93E-01
Max	9.72	1.49E+01	1.16E-10	2.06E+00	4.01E+00	8.95E+00	3.34E-01	6.25E+00	2.50E-03	9.90E+00	1.07E+01	1.87E+00	3.01E-01	3.18E+01
s	1.12	8.88E-01	6.07E-12	5.39E-01	6.34E-01	1.21E+00	1.08E-01	1.09E+00	3.89E-04	1.94E+00	1.41E+00	3.81E-01	6.51E-02	5.72E+00
2s	2.23	1.78E+00	1.21E-11	1.08E+00	1.27E+00	2.42E+00	2.17E-01	2.17E+00	7.78E-04	3.87E+00	2.82E+00	7.61E-01	1.30E-01	1.14E+01

Source: Output DTN: MO0310SPAEBSCB.003.

NOTE: All units, except pH and Cl:NO₃, are in moles/kg×H₂O.

Table 6.6-8. Bin Map for "Water 0" Incoming Seepage Waters

Start (yr)	End (yr)	Bin for Invert Seepage (w0bf4)	Bin for Crown Seepage (w0tf4)	EQ6 Output Filename
0	50	4	4	10.6o
50	52	5	5	51.6o
52	54	11	5	53.6o
54	57.5	11	6	55.6o
57.5	67.5	2	6	60.6o
67.5	87.5	1	5	75.6o
87.5	125	1	5	100.6o
125	175	2	4	150.6o
175	225	2	4	200.6o
225	275	2	3	250.6o
275	325	2	3	300.6o
325	375	2	3	350.6o
375	450	2	3	400.6o
450	550	2	4	500.6o
550	625	3	4	600.6o
625	675	3	5	650.6o
675	725	4	11	700.6o
725	769.5	4	11	750.6o
769.5	794.5	4	11	789.6o
794.5	900	4	11	800.6o
900	1,100	5	11	1000.6o
1,100	1,300	5	11	1200.6o
1,300	1,500.5	5	11	1400.6o
1,500.5	1,701	5	11	1601.6o
1,701	1,901	5	11	1801.6o
1,901	2,101	9	4	2001.6o
2,101	2,301	11	11	2201.6o
2,301	2,701.5	11	11	2401.6o
2,701.5	4,002.5	11	11	3002.6o
4,002.5	6,003.5	11	11	5003.6o
6,003.5	8,505	6	6	7004.6o
8,505	11,158	7	6	10006.6o
11,158	13,660	7	7	12310.6o
13,660	17,511.5	7	7	15010.6o
17,511.5	35,023.5	8	8	20013.6o
35,023.5	100,000	8	8	50034.6o

Source: Output DTN: MO0310SPAEBSCB.003.

Table 6.6-9. Bin Map for "Water 4" Incoming Seepage Waters

Start (Yr)	End (Yr)	Bin for Invert Seepage (w4bf4)	Bin for Crown Seepage (w4tf4)	EQ6 Output Filename
0	50	10	10	10.6o
50	52	11	11	51.6o
52	54	11	11	53.6o
54	57.5	11	11	55.6o
57.5	67.5	4	11	60.6o
67.5	87.5	11	11	75.6o
87.5	125	11	11	100.6o
125	175	4	11	150.6o
175	225	4	11	200.6o
225	275	5	11	250.6o
275	325	4	11	300.6o
325	375	5	11	350.6o
375	450	5	11	400.6o
450	550	4	5	500.6o
550	625	4	5	600.6o
625	675	4	11	650.6o
675	725	5	11	700.6o
725	775	5	11	750.6o
775	802	11	11	800.6o
802	902	11	11	804.6o
902	1,100	11	11	1000.6o
1,100	1,300	11	11	1200.6o
1,300	1,500.5	11	11	1400.6o
1,500.5	1,701	11	11	1601.6o
1,701	1,901	11	5	1801.6o
1,901	2,101	11	4	2001.6o
2,101	2,301	11	11	2201.6o
2,301	2,499	11	11	2401.6o
2,499	2,799.5	11	11	2597.6o
2,799.5	4,002.5	11	11	3002.6o
4,002.5	6,003.5	11	11	5003.6o
6,003.5	8,505	9	9	7004.6o
8,505	11,301.5	7	7	10006.6o
11,301.5	13,803.5	7	7	12597.6o
13,803.5	17,511.5	8	8	15010.6o
17,511.5	35,023.5	8	8	20013.6o
35,023.5	100,000	8	8	50034.6o

Source: Output DTN: MO0310SPAEBSCB.003.

Table 6.6-10. Bin Map for "Water 5" Incoming Seepage Waters

Start (yr)	End (yr)	Bin for Invert Seepage (w5bf4)	Bin for Crown Seepage (w5tf4)	EQ6 Output Filename
0	50	7	7	10.6o
50	52	11	11	51.6o
52	54	11	11	53.6o
54	57.5	11	11	55.6o
57.5	67.5	3	11	60.6o
67.5	87.5	4	11	75.6o
87.5	125	2	11	100.6o
125	175	4	11	150.6o
175	225	4	11	200.6o
225	275	5	11	250.6o
275	325	4	11	300.6o
325	375	4	11	350.6o
375	450	4	11	400.6o
450	550	4	9	500.6o
550	625	5	11	600.6o
625	675	5	11	650.6o
675	725	11	11	700.6o
725	767	11	11	750.6o
767	792	11	11	784.6o
792	900	11	11	800.6o
900	1,100	11	11	1000.6o
1,100	1,300	11	11	1200.6o
1,300	1,500.5	11	11	1400.6o
1,500.5	1,701	11	11	1601.6o
1,701	1,901	11	5	1801.6o
1,901	2,101	11	4	2001.6o
2,101	2,296.5	11	11	2201.6o
2,296.5	2,396.5	11	11	2392.6o
2,396.5	2,701.5	11	11	2401.6o
2,701.5	4,002.5	11	11	3002.6o
4,002.5	6,003.5	11	11	5003.6o
6,003.5	8,505	9	9	7004.6o
8,505	11,155	10	10	10006.6o
11,155	13,657	7	7	12304.6o
13,657	17,511.5	7	7	15010.6o
17,511.5	35,023.5	8	8	20013.6o
35,023.5	100,000	8	8	50034.6o

Source: Output DTN: MO0310SPAEBSCB.003.

Table 6.6-11. Bin Map for "Water 6" Incoming Seepage Waters

Start (yr)	End (yr)	Bin for Invert Seepage (w6bf4)	Bin for Crown Seepage (w6tf4)	EQ6 Output Filename
0	50	7	7	10.6o
50	52	9	9	51.6o
52	54	9	9	53.6o
54	57.5	9	9	55.6o
57.5	67.5	2	9	60.6o
67.5	87.5	1	9	75.6o
87.5	125	2	9	100.6o
125	175	4	9	150.6o
175	225	4	9	200.6o
225	275	9	9	250.6o
275	325	4	9	300.6o
325	375	4	9	350.6o
375	450	9	9	400.6o
450	550	4	6	500.6o
550	625	4	9	600.6o
625	675	9	9	650.6o
675	725	9	9	700.6o
725	775	9	9	750.6o
775	832.5	9	9	800.6o
832.5	932.5	9	9	865.6o
932.5	1,100	9	9	1000.6o
1,100	1,300	9	9	1200.6o
1,300	1,500.5	9	9	1400.6o
1,500.5	1,701	9	9	1601.6o
1,701	1,901	9	6	1801.6o
1,901	2,101	9	4	2001.6o
2,101	2,301	9	9	2201.6o
2,301	2,701.5	9	9	2401.6o
2,701.5	3,025	9	9	3002.6o
3,025	4,025.5	9	9	3048.6o
4,025.5	6,003.5	9	9	5003.6o
6,003.5	8,505	9	9	7004.6o
8,505	11,529.5	10	10	10006.6o
11,529.5	14,031.5	10	10	13053.6o
14,031.5	17,511.5	10	10	15010.6o
17,511.5	35,023.5	8	8	20013.6o
35,023.5	100,000	8	8	50034.6o

Source: Output DTN: MO0310SPAEBSCB.003.

Table 6.6-12. Bin Map for "Water 7" Incoming Seepage Waters

Start (yr)	End (y)	Bin for Invert Seepage (w7bf4)	Bin for Crown Seepage (w7tf4)	EQ6 Output Filename
0	50	7	7	10.6o
50	52	11	11	51.6o
52	54	11	11	53.6o
54	57.5	11	11	55.6o
57.5	67.5	3	11	60.6o
67.5	87.5	1	11	75.6o
87.5	125	2	11	100.6o
125	175	4	11	150.6o
175	225	4	11	200.6o
225	275	4	11	250.6o
275	325	3	5	300.6o
325	375	3	4	350.6o
375	450	3	4	400.6o
450	550	2	4	500.6o
550	625	3	4	600.6o
625	675	4	5	650.6o
675	725	4	11	700.6o
725	767	4	11	750.6o
767	792	5	11	784.6o
792	900	5	11	800.6o
900	1,100	6	11	1000.6o
1,100	1,300	11	11	1200.6o
1,300	1,500.5	11	11	1400.6o
1,500.5	1,701	11	11	1601.6o
1,701	1,901	11	11	1801.6o
1,901	2,101	11	11	2001.6o
2,101	2,301	11	11	2201.6o
2,301	2,496	11	11	2401.6o
2,496	2,796.5	11	11	2591.6o
2,796.5	4,002.5	11	11	3002.6o
4,002.5	6,003.5	11	11	5003.6o
6,003.5	8,505	9	9	7004.6o
8,505	11,301	7	7	10006.6o
11,301	13,803	7	7	12596.6o
13,803	17,511.5	7	7	15010.6o
17,511.5	35,023.5	8	8	20013.6o
35,023.5	100,000	8	8	50034.6o

Source: Output DTN: MO0310SPAEBSCB.003.

6.6.7 Impact Analysis Due to Errors Identified in AP-SIII.10Q 5.4.3

The binning process has been developed to facilitate an evaluation of whether any new input (such as a new THC seepage model output) would require a new type of chemistry (i.e., a new bin) that this abstraction has not investigated. Only if a potential water falls outside a defined bin area is reanalysis of potential seepage compositions necessary. The 11 bins are designed to cover a broad range of possible water chemistry within the drift. Likewise, if an error is found in the calculated chemistries, and an analysis of the error finds that the corrected chemistry falls within the same bin, then there is no real impact to the chemistries within that bin (i.e., the predicted evolution of the chemistry in the bin does not change), so the current median water is still sufficient to represent the corrected water.

During the check process, two errors in the binning abstraction were discovered. The first dealt with four of the 368 input waters not being completely normalized to an activity of water equaling 0.65. This occurred when the number of iterations EQ6 was allowed to perform was set too low for the calculation to reach the desired activity of water (a_w). The second error occurred when the $p\text{CO}_2$ inputs used from the five THC seepage model outputs were not converted from dimensionless volume fractions to partial pressures in bars. Thus, the volume fractions in the model runs used for the binning process were treated as if they were partial pressures in bars. The impact evaluation of these two errors resulted in no changes to the assigned bins; therefore, these errors have no impact on the lookup tables developed in Section 6.9. The details of the impact analyses are documented in the following section.

6.6.7.1 Endpoint a_w

Table 6.6-13 lists the files that do not normalize to an a_w of 0.65 and the results of the recalculation down to an a_w of 0.65.

Table 6.6-13. Details of Impact Analysis on Binning Due to Endpoint a_w

Water/File Name ^a	Initial Endpoint a_w ^b	Initial Bin ^b	New Endpoint a_w ^c	New Bin ^c
W4bf4 2597.6o	0.72	11	0.65	11
W4bf4 3002.6o	0.706	11	0.65	11
W5bf4 3002.6o	0.695	11	0.65	11
W6bf4 3002.6o	0.675	9	0.65	9

Sources: ^a Output DTN: MO0303MWDEBSSM.000.

^b Output DTN: MO0310SPAEBSCB.003; *Final Checked EBS THC Seepage Binning Abstraction Rev 4.xls*.

^c Output DTN: MO0310SPAEBSCB.003; *Bin Abstraction Rerun.xls*.

These four files were rerun to the correct water activity and the binning criteria discussed in Section 6.6.4 were reapplied. All of the waters fell within the original bins. Therefore, there was no impact to the lookup tables developed in Section 6.9. All recalculated EQ6 files and the rebinning spreadsheet (*Bin Abstraction Rerun.xls*) are archived in DTN: MO0310SPAEBSCB.003.

6.6.7.2 CO₂ Pressure Correction

To evaluate the impact of the error in units for the fugacity of CO₂, the median waters that are determined to represent the eleven bins were rerun with corrected CO₂ fugacity. The fugacity was corrected by multiplying the original volume fractions by the approximate average total atmospheric pressure at Yucca Mountain of between 0.88 and 0.89 bars (*gas flux.xls*, tab "fractures-ch" archived in DTN: MO0308SPAPCEGF.001). This action converts the volume fractions to partial pressures in bars.

After reapplying the binning criteria discussed in Section 6.6.4, all of the waters fall within the same bin as the original calculation runs (Table 6.6-14), showing that the error in the $p\text{CO}_2$ values has no effect on the binning analysis. All recalculated EQ6 files and the rebinning spreadsheet (*Bin Abstraction Rerun.xls*) are archived in output DTN: MO0310SPAEBSCB.003.

Table 6.6-14. Details of Impact Analysis on CO₂ Pressure Correction

Water/File Name ^a	Initial log CO ₂ Value ^b	Initial Bin ^b	Corrected log CO ₂ Value ^c	New Bin ^c
W7bf4/75.6o	-3.41	1	-3.466	1
W0bf4/250.6o	-3.307	2	-3.363	2
W0bf4/650.6o	-2.984	3	-3.040	3
W4bf4/600.6o	-3.312	4	-3.368	4
W7tf4/300.6o	-2.726	5	-2.782	5
W0tf4/7004.6o	-2.151	6	-2.207	6
W4bf4/10006.6o	-1.926	7	-1.982	7
W5tf4/20013.6o	-2.198	8	-2.254	8
W6tf4/51.6o	-2.532	9	-2.589	9
W5bf4/10006.6o	-2.037	10	-2.093	10
W4tf4/300.6o	-2.392	11	-2.448	11

Sources: ^a Output DTN: MO0303MWDEBSSM.000.

^b Output DTN: MO0310SPAEBSCB.003; *Final Checked EBS THC Seepage Binning Abstraction Rev 4.xls*.

^c Output DTN: MO0310SPAEBSCB.003; *Bin Abstraction Rerun.xls*.

6.7 EVOLUTION OF IN-DRIFT GAS AND TEMPERATURE

The purposes of this section are:

- To analyze oxygen demand in the drift. This determines the potential (given the large masses of introduced materials in the drift) for the development of oxygen-deficient conditions.
- To establish the expected range of $p\text{CO}_2$ through time and derive lookup tables for this parameter for the TSPA-LA
- To establish the expected range of in-drift temperatures, for use in developing lookup tables
- To report values of trace gas fugacity in equilibrium with the initial THC seepage and dust leachate waters used as inputs to this model.

6.7.1 Oxygen Evaluation

Two evaluations of the in-drift oxygen are reported here as part of the gas abstraction model. The first is a simple examination of the THC seepage model results that is used to directly calculate in-drift oxygen partial pressure and accounts for air displacement resulting from thermal water-vapor generation. The second involves a mass balance calculation that estimates a steady-state oxygen partial pressure by balancing the oxygen flux (as given by the THC seepage model) with oxygen consumption due to corrosion.

6.7.1.1 THC Air Fraction

The in-drift fraction of air is available in the THC seepage model output DTN: LB0302DSCPTHCS.002 within the five files titled *thc6_w#_drift_r.xls* (where # is 0 and 4 through 7) and under Tab "fracture-th," columns labeled "Xair Crown." These are plotted together in Figure 6.7-1.

The minimum value from all available air fraction data, at all drift wall locations (crown, side, and base) is 3.5×10^{-5} (unitless air fraction). Multiply that with the resulting oxygen fraction (multiply air fraction by 0.21 fraction of oxygen in air, Table 4.1-16) and the pressure at the repository level (0.89 bars) to obtain a THC seepage model minimum oxygen content of 6.5×10^{-6} bars (for these results see output DTN: SN0407T0510102.017, *Air fraction.xls*).

Source DTN: LB0302DSCPTHC5.002.

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 CO_2 generation as compared to flux, O_2 consumption (the same reaction generating CO_2) 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 169856]). 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 169856]).

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.

Output DTN: SN0407T0510102.017.

NOTE: Time = 50 years represents the time at which forced ventilation stops.

Figure 6.7-2. Gas Flux per Axial Meter of Drift per Year

The second step in the mass balance is to calculate the oxygen consumption rate of the low-alloy steels in the introduced materials as they corrode for two cases:

- Corrosion of materials outside of the waste package
- Corrosion of commercial waste packages (21-PWR).

Consideration is only given to the carbon or low-alloy steel components. This is because of their large mass and dominant corrosion rate (Table 6.4-18), making the carbon/low-alloy steels the only materials to consume oxygen at a significant rate due to corrosion. A ratio of 1.5 moles of oxygen atoms per mole of iron is used based on the formation of any ferric iron (Fe^{3+}) solid or aqueous product. This ratio is also a maximum for iron oxidation and therefore consumes the most oxygen.

Invert Material Corrosion—The materials inside the waste package are not expected to corrode until the corrosion-resistant (Alloy 22) outer shell is breached, long after the end of the regulatory period. However, the corrosion of materials in the waste package is included in the oxygen consumption calculations as an upper bound of oxygen consumption. Using the size specifications from Table 4.1-10 to determine the surface area and the corrosion rate for low-alloy or carbon (steam and atmospheric) listed in Table 6.4-18 (justified within Section 4.1.2), the oxygen consumption rate due to corrosion of all low-alloy or carbon steel materials

outside the waste package (invert and gantry rail) is calculated (DTN: SN0407T0510102.017, *Oxygen Demand.xls*, tab "Invert O2 Consumption").

The unrestricted oxygen demand from this invert material corrosion is 235 mol/yr-m of oxygen (470 mol/yr-m of oxygen atoms). In the linear steady-state relation, where oxygen consumption must equal demand, the demand will decrease to 3 mol/yr-m (6 mol/yr-m oxygen atom consumed). Therefore, the relative level to which the oxygen pressure decreases is simply the ratio of supply to demand (6 divided by 471). This relative oxygen content is then multiplied by the pressure of oxygen in air (approximately 0.21, Table 4.1-16) to give the oxygen partial pressure; this value need not be adjusted for the repository level pressures as they are based upon the corrosion experiments that primarily occurred near sea level. The results indicate that due to the invert and gantry rail steel emplacements within the drift, the oxygen pressure may drop to approximately 2.7×10^{-3} bars.

Waste Package Material Corrosion—Once the waste package itself is breached, materials in the package may begin to undergo oxygen-mediated corrosion. Oxygen partial pressure is modeled with the conservative simplification that an entire drift consisting of 21-PWR waste packages ruptures simultaneously. Using the surface areas in Table 4.1-17 (Source DTN: MO0210MWDEXC01.008 [DIRS 163531], *CSNF WP Model Abstraction.xls*) for the 21-PWR internal low-alloy/carbon steel materials, oxygen consumption rates are calculated and the steady-state partial pressure of oxygen estimated (output DTN: SN0407T0510102.017, *Oxygen Demand.xls*, tab "21-PWR O2 Consumption"). Although of high surface area, the waste material itself was not considered in this modeling as it is encased in Zircaloy; this will prevent all the fuel from being exposed at the same time.

The unrestricted oxygen demand from corrosion of material within the waste package is 937 mol/yr-m of oxygen (1,874 mol/yr-m of oxygen atoms). Comparison to the oxygen flux of 3 mol/yr-m is similar to that for the invert. This example involving the entire failure of a drift containing only the 21-PWR waste packages leads to a lower oxygen pressure of 6.8×10^{-4} bars.

6.7.1.3 Comparison to Important Redox Couples

All of these oxygen levels from Sections 6.7.1.1 and 6.7.1.2 are still well above those required to produce anoxic conditions. To demonstrate this, three EQ3/6 calculations are performed to determine the following:

- Nitrate/nitrite equivalence point oxygen pressure
- Approximate ferric/ferrous iron equivalence point oxygen pressure
- Various redox species present at the minimum drift oxygen pressure.

These calculations are contained in the output DTN: SN0407T0510102.017 in the input/output files, corresponding to the list above: *no2no3.3i/.3o*, *fe2fe3.3i/.3o*, and *minoxy.3i/.3o*.

The nitrate–nitrite couple was calculated using the Pitzer thermodynamic database (DTN: SN0302T0510102.002 [DIRS 162572]). The equivalence point, where NO_3^- equals NO_2^- in solution, is calculated to be at an oxygen pressure of 2.7×10^{-28} bars.

The ferric-ferrous couple was calculated using the *data0.ymp.R2* B-dot database (DTN: MO0302SPATHDYN.000 [DIRS 161756]) because the Pitzer database is not validated for iron speciation. The near-equivalence point, first two iron species are $\text{HFeO}_{2(\text{aq})} = 4.3 \times 10^{-11}$ and $\text{Fe}^{2+} = 3.3 \times 10^{-11}$, is calculated to be at an oxygen pressure of 1.4×10^{-54} bars.

An alternate analysis is to compare the calculated quantity of redox species found at the lowest reasonably expected oxygen pressure from the determinations in Sections 6.7.1.1 and 6.7.1.2. This is at the THC Seepage Model's minimum air fraction result at 6.5×10^{-6} bars. The results show that at such an oxygen pressure, with Fe^{3+} species at the 10^{-10} molal level, the Fe^{2+} is less than the 10^{-22} molal. Aqueous hydrogen peroxide is in the same range at 2×10^{-21} molal.

These three comparisons all indicate that the minimum oxygen pressures expected within the in-drift environment are all sufficient to prevent anoxic conditions from occurring.

6.7.2 Thermal-Hydrological-Chemical Seepage Model In-Drift CO_2 Gas and Temperature Abstraction

The $p\text{CO}_2$ and temperature in the drift environment can affect chemical processes, such as radionuclide solubility. As an illustration, the uranium concentration in equilibrium with schoepite ($\text{UO}_3 \cdot 2\text{H}_2\text{O}$) is shown to be at least ten times higher for $p\text{CO}_2 = 10^{-2}$ bar compared to $p\text{CO}_2 = 0$ for $\text{pH} > 7$ (Langmuir 1997 [DIRS 100051], Figure 13.5). Section 6.7.2.1 provides the lookup tables for in-drift and invert $p\text{CO}_2$ values, which correspond to the seepage compositions presented in Section 6.6.5. Section 6.7.2.2 provides a range of values of $p\text{CO}_2$ and temperatures for construction of water chemistry lookup tables presented in Section 6.9.3.

6.7.2.1 Total Systems Performance Assessment - License Application Lookup Tables for Drift and Invert $p\text{CO}_2$

In conjunction with the seepage binning and bin maps presented in Section 6.6.6 (Tables 6.6-8 to 6.6-12), the TSPA-LA requires lookup tables to constrain the $p\text{CO}_2$ within the drift and invert for each of the five seepage compositions (Section 4.1.3).

These lookup tables (Tables 6.7-1 to 6.7-5) are prepared using the ten THC seepage model output files listed in Table 4.1-14. The tables are found in *THC CO2 GAS & TEMP COMPARE.xls* (archived in output DTN: MO0308SPACO2GL.001). The file types *thc6_XX_drift_r.xls* (where XX is the abbreviated water name) are the source of the in-drift values; and the file types *thc6_XX_r.xls* are the source for the invert values. The in-drift values represent the $p\text{CO}_2$ values at the crown taken from worksheet "fracture-ch." The invert values represent the $p\text{CO}_2$ with the following designations: quadrant = bottom, zone = front, worksheet = "matrix-ch", index = 4. The $p\text{CO}_2$ values are plotted as a function of time in Figures 6.7-5 and 6.7-6. Figure 6.7-5 is a log-log plot of all the values; whereas, Figure 6.7-6 is a linear plot of the in-drift values only. The atmospheric $p\text{CO}_2$ (Weast and Astle 1979 [DIRS 102865], p. F-211) is also plotted for reference purposes. Both figures show the $p\text{CO}_2$ values for various spatial locations, namely, within the drift, in the rock near the drift wall crown, and near the base of the invert.

(Figures 6.7-3 and 6.7-4 intentionally deleted.)

Output DTN: MO0308SPACO2GL001.

NOTES: See Table 4.1-13 for abbreviated water names of labels in the legend.

Units for $p\text{CO}_2$ in bars.

Units for time in years.

Figure 6.7-5. $p\text{CO}_2$ Concentration in the Drift and Near-Drift Environment Through Time (Log Scale)

Output DTN: MO0308SPACO2GL001.

NOTES: See Table 4.1-13 for abbreviated water names of labels in the legend.

Units for $p\text{CO}_2$ in bars.

Units for time in years.

Figure 6.7-6. $p\text{CO}_2$ Concentration in the In-Drift Environment Through Time (Normal Scale)

6.7.2.2 CO₂ and Temperature Values for Construction of Water Chemistry Abstraction Lookup Tables

The intent of the in-drift seepage evaporation abstraction (Section 6.9) is to take the 11 bin water values abstracted in Section 6.6 and calculate the resulting composition after evaporation or dilution using the in-drift precipitates salts model to generate lookup tables for use in the TSPA-LA. For the evaporation calculations, ranges of temperature and carbon dioxide fugacity are needed to capture the effects of these parameters on the evaporative evolution.

To determine the $p\text{CO}_2$ range, $p\text{CO}_2$ values presented in *THC CO2 GAS & TEMP COMPARE.xls* (output DTN: MO0308SPACO2GL.001) were statistically analyzed using the built-in functions in the Microsoft Excel 97 software application. The overall fugacity ranges from a maximum of 1.75×10^{-2} bar (CS500, invert) to a minimum of 2.29×10^{-5} bar (HD-Perm, in-drift). The median value is determined to be 3.01×10^{-3} bar. The majority of values fall between 1.0×10^{-4} and 1.0×10^{-2} bar and only six values fall below 1.0×10^{-4} bar, or about 0.82 percent of all data points. The upper limit, or 95th percentile, value for all data points is 8.8×10^{-3} bar. Based on the statistical analysis, the three values selected for use are 1.0×10^{-2} , 1.0×10^{-3} , and 1.0×10^{-4} bar. Sensitivity cases have been run using a larger range of $p\text{CO}_2$ (Section 6.12.4.3) to demonstrate that this larger range can be reached by extrapolation.

The in-drift temperature range (Figure 6.7-7) is constructed using the following four time-temperature curves: the waste package node, the drift wall surface at the crown of the drift, the base of invert, and within the rock above the crown of the drift (output DTN: MO0308SPACO2GL.001, *THC CO2 GAS & TEMP COMPARE.xls*). The plotted curves of Figure 6.7-7 indicate that the minimum temperature in the drift after 20,000 years is 40°C. The maximum in-drift temperature can be as great as approximately 180°C on the waste package surface and 150°C at the drift wall during the peak thermal pulse (BSC 2004 [DIRS 169565], Figure 6.3-2).

An evaluation of the THC model output in Figure 6.7-7 shows that only in the period from 50 to approximately 2,000 years are the temperatures above 100°C, which is the time when liquid water available for macroscale reaction is limited by the temperature pulse in the drift (Figure 6.2-4). Accurate modeling is also limited to temperatures of right around 100°C or less because of the limits imposed by the boiling point at the elevation of the drift, uncertainties in the boiling point elevation due to concentration of porewater salts, and temperature limitations on the applicability of some thermodynamic data in the *Data0.yfp* database (DTN: SN0302T0510102.002 [DIRS 162572]). Therefore, an upper calculation limit of 100°C is within an acceptable range of calculational uncertainty.

For the infrequent and brief events where seepage occurs onto surfaces slightly above 100°C, the results at 100°C are used as an extrapolation. At the most, when the drift wall cools through 100°C, the waste package temperatures are at or below 110°C (BSC 2004 [DIRS 169565], Figure 6.3-14). The effect of this higher temperature extrapolation on the equilibrium seepage modeling will be upon the log K values. The solubilities the most soluble minerals of relevance at such temperatures typically all increase and thereby cancel out any net effect upon the relative seepage composition. Therefore, this extrapolation of 100°C results above this to the temperature of the waste package is reasonable.

With these upper and lower bounds, the midpoint between these two bounding points is selected (70°C). The three temperatures (40°C, 70°C, and 100°C) are used to construct the lookup tables for use in the analyses described in the following section and for the construction of the lookup tables for the TSPA-LA.

Output DTN: MO0308SPACO2GL001.

Figure 6.7-7. Comparison of Temperatures at Various Locations Within and Around the Drift as Determined by the Thermal-Hydrological-Chemical Model Output

Table 6.7-1. Lookup Tables for Total System Performance Assessment-License Application Analysis of In-Drift and Invert $p\text{CO}_2$ for W0 (HD-PERM) Seepage Water

w0, HD-PERM		Drift	Invert
Start (yr)	End (yr)	Partial Pressure $\text{CO}_{2(g)}$ bars	Partial Pressure $\text{CO}_{2(g)}$ bars
1.00	2.50	1.21E-03	2.43E-03
2.50	7.50	1.12E-03	1.58E-03
7.50	15.00	1.05E-03	1.26E-03
15.00	25.00	9.51E-04	9.89E-04
25.00	35.00	8.82E-04	9.39E-04
35.00	45.00	8.80E-04	1.01E-03
45.00	50.50	8.61E-04	9.54E-04
50.50	52.00	4.25E-04	1.69E-03
52.00	54.00	1.86E-04	1.04E-03
54.00	56.00	1.01E-04	5.13E-04
56.00	61.00	2.29E-05	7.82E-04
61.00	71.50	8.25E-05	1.32E-04
71.50	101.50	2.29E-04	2.53E-04
101.50	150.00	4.58E-04	4.75E-04
150.00	200.00	5.28E-04	5.53E-04
200.00	250.00	4.34E-04	4.34E-04
250.00	300.00	3.18E-04	3.20E-04
300.00	350.00	2.60E-04	2.49E-04
350.00	412.50	2.60E-04	2.39E-04
412.50	500.00	3.93E-04	3.68E-04
500.00	588.50	7.12E-04	6.85E-04
588.50	651.00	9.97E-04	9.14E-04
651.00	713.00	1.30E-03	1.22E-03
713.00	770.00	1.65E-03	1.58E-03
770.00	795.00	1.85E-03	1.84E-03
795.00	900.50	2.02E-03	1.99E-03
900.50	1,100.50	3.63E-03	3.59E-03
1,100.50	1,301.00	4.61E-03	4.62E-03
1,301.00	1,501.00	5.60E-03	5.57E-03
1,501.00	1,701.00	6.32E-03	6.32E-03
1,701.00	1,901.50	6.81E-03	6.79E-03
1,901.50	2,101.50	6.51E-03	6.29E-03
2,101.50	2,301.50	7.10E-03	8.81E-03
2,301.50	2,401.50	7.49E-03	1.03E-02
2,401.50	2,702.00	7.97E-03	1.52E-02
2,702.00	4,003.00	7.20E-03	8.28E-03
4,003.00	6,004.00	6.08E-03	7.20E-03
6,004.00	8,505.50	6.22E-03	6.69E-03
8,505.50	11,158.50	6.31E-03	6.04E-03
11,158.50	13,660.00	5.90E-03	5.16E-03
13,660.00	17,511.50	5.21E-03	3.81E-03
17,511.50	100,000.00	4.02E-03	2.02E-03

Source: Output DTN: MO0308SPACO2GL.001.

Table 6.7-2. Lookup Tables for Total System Performance Assessment-License Application Analysis of In-Drift and Invert $p\text{CO}_2$ for W4 (CS2000) Seepage Water

w4, CS2000		Drift	Invert
Start (yr)	End (yr)	Partial Pressure $\text{CO}_{2(g)}$ bars	Partial Pressure $\text{CO}_{2(g)}$ bars
1.00	2.50	3.75E-03	5.27E-03
2.50	7.50	4.11E-03	5.11E-03
7.50	15.00	3.97E-03	4.42E-03
15.00	25.00	3.79E-03	3.78E-03
25.00	35.00	3.75E-03	3.73E-03
35.00	45.00	3.82E-03	3.89E-03
45.00	50.00	3.87E-03	3.92E-03
50.00	52.00	2.31E-03	8.78E-03
52.00	54.00	8.59E-04	3.96E-03
54.00	57.50	5.25E-04	2.44E-03
57.50	65.00	8.70E-05	3.60E-04
65.00	77.50	3.97E-04	5.05E-04
77.50	125.00	1.32E-03	1.51E-03
125.00	175.00	3.05E-03	3.22E-03
175.00	225.00	4.09E-03	4.20E-03
225.00	275.00	4.01E-03	4.07E-03
275.00	325.00	3.37E-03	3.39E-03
325.00	375.00	2.63E-03	2.65E-03
375.00	450.00	1.89E-03	1.89E-03
450.00	550.00	8.05E-04	8.01E-04
550.00	625.00	4.50E-04	4.29E-04
627.00	675.00	5.54E-04	5.02E-04
675.00	725.00	6.80E-04	6.31E-04
725.00	775.00	9.65E-04	8.85E-04
775.00	802.00	1.24E-03	1.18E-03
802.00	900.00	1.24E-03	1.19E-03
900.00	1,100.00	2.98E-03	2.95E-03
1,100.00	1,300.00	4.63E-03	4.61E-03
1,300.00	1,500.50	5.69E-03	5.64E-03
1,500.50	1,700.50	6.48E-03	6.43E-03
1,700.50	1,900.50	6.55E-03	6.57E-03
1,900.50	2,100.50	6.60E-03	6.64E-03
2,101.50	2,300.50	7.47E-03	8.62E-03
2,300.50	2,498.00	7.89E-03	1.05E-02
2,498.00	2,701.00	6.96E-03	1.74E-02
2,701.00	4,002.50	7.82E-03	1.44E-02
4,002.50	6,003.50	7.63E-03	1.03E-02
6,003.50	8,505.00	8.55E-03	1.00E-02
8,505.00	11,301.50	9.87E-03	1.05E-02
12,597.90	13,804.50	1.01E-02	1.05E-02
15,010.10	17,511.50	9.63E-03	9.85E-03
17,511.50	100,000.00	8.19E-03	8.18E-03

Source: Output DTN: MO0308SPACO2GL.001.

Table 6.7-3. Lookup Tables for Total System Performance Assessment-License Application Analysis of In-Drift and Invert $p\text{CO}_2$ for W5 (CS1000) Seepage Water

w5, CS1000		Drift	Invert
Start (yr)	End (yr)	Partial Pressure $\text{CO}_{2(g)}$ bars	Partial Pressure $\text{CO}_{2(g)}$ bars
1.00	2.50	3.73E-03	4.06E-03
2.50	7.50	3.00E-03	3.18E-03
7.50	15.00	2.75E-03	3.00E-03
15.00	25.00	2.50E-03	2.54E-03
25.00	35.00	2.35E-03	2.41E-03
35.00	45.00	2.31E-03	2.50E-03
45.00	50.50	2.26E-03	2.39E-03
50.50	52.00	1.12E-03	5.20E-03
52.00	54.00	4.47E-04	2.91E-03
54.00	57.50	2.82E-04	1.49E-03
57.50	67.50	8.33E-05	2.78E-04
67.50	87.50	2.10E-04	2.60E-04
87.50	125.00	6.49E-04	7.44E-04
125.00	175.00	1.47E-03	1.54E-03
175.00	225.00	1.85E-03	1.89E-03
225.00	275.00	1.67E-03	1.69E-03
275.00	325.00	1.29E-03	1.29E-03
325.00	375.50	9.04E-04	9.05E-04
375.50	450.50	5.82E-04	5.73E-04
450.50	550.50	3.27E-04	3.05E-04
550.50	625.50	4.86E-04	4.50E-04
625.50	675.50	7.01E-04	6.38E-04
675.50	725.50	9.52E-04	9.07E-04
725.50	767.50	1.28E-03	1.23E-03
767.50	792.50	1.52E-03	1.49E-03
792.50	900.50	1.70E-03	1.66E-03
900.50	1,100.50	3.36E-03	3.28E-03
1,100.50	1,301.00	4.40E-03	4.41E-03
1,301.00	1,501.00	5.49E-03	5.50E-03
1,501.00	1,701.00	6.30E-03	6.34E-03
1,701.00	1,901.50	6.50E-03	6.52E-03
1,901.50	2,101.50	6.59E-03	6.70E-03
2,101.50	2,297.00	7.33E-03	8.32E-03
2,297.00	2,397.00	7.66E-03	9.40E-03
2,397.00	2,702.00	7.75E-03	1.00E-02
2,702.00	4,003.00	7.11E-03	1.56E-02
4,003.00	6,004.00	6.78E-03	9.75E-03
6,004.00	8,505.50	7.10E-03	8.56E-03
8,505.50	11,155.50	7.55E-03	8.11E-03
11,155.50	13,657.00	7.42E-03	7.72E-03
13,657.00	17,511.50	6.83E-03	6.93E-03
17,511.50	100,000.00	5.59E-03	5.54E-03

Source: Output DTN: MO0308SPACO2GL.001.

Table 6.7-4. Lookup Tables for Total System Performance Assessment-License Application Analysis of In-Drift and Invert $p\text{CO}_2$ for W6 (SD-9) Seepage Water

w6, SD-9		Drift	Invert
Start (yr)	End (yr)	Partial Pressure $\text{CO}_{2(g)}$ bars	Partial Pressure $\text{CO}_{2(g)}$ bars
1.00	2.50	3.36E-03	6.03E-03
2.50	7.50	3.81E-03	4.94E-03
7.50	15.00	3.77E-03	4.06E-03
15.00	25.00	3.69E-03	3.57E-03
25.00	35.00	3.73E-03	3.62E-03
35.00	45.00	3.82E-03	3.81E-03
45.00	50.50	3.88E-03	3.86E-03
50.50	52.00	1.99E-03	1.14E-02
52.00	54.00	7.56E-04	2.98E-03
54.00	57.54	4.48E-04	1.35E-03
57.54	67.55	9.07E-05	3.82E-04
67.55	87.56	3.26E-04	4.10E-04
87.56	125.08	9.72E-04	1.11E-03
125.08	175.00	1.76E-03	1.85E-03
175.00	225.00	1.98E-03	2.02E-03
225.00	275.00	1.69E-03	1.71E-03
275.00	325.00	1.22E-03	1.23E-03
325.00	375.00	8.07E-04	8.11E-04
375.00	450.50	4.89E-04	4.86E-04
450.50	550.50	2.50E-04	2.28E-04
550.50	625.50	4.10E-04	3.78E-04
625.50	675.50	6.09E-04	5.49E-04
675.50	725.50	8.76E-04	8.09E-04
725.50	775.50	1.18E-03	1.14E-03
775.50	833.00	1.60E-03	1.54E-03
833.00	933.00	2.08E-03	2.07E-03
933.00	1,100.50	3.04E-03	3.03E-03
1,100.50	1,301.00	4.22E-03	4.23E-03
1,301.00	1,501.00	5.38E-03	5.34E-03
1,501.00	1,701.00	6.21E-03	6.20E-03
1,701.00	1,901.50	6.41E-03	6.47E-03
1,901.50	2,101.50	6.47E-03	6.58E-03
2,101.50	2,301.50	7.05E-03	7.68E-03
2,301.50	2,702.00	7.41E-03	9.13E-03
2,702.00	3,025.00	6.95E-03	1.66E-02
3,025.00	4,026.02	6.38E-03	1.63E-02
4,026.02	6,004.00	5.92E-03	8.98E-03
6,004.00	8,505.50	5.98E-03	7.25E-03
8,505.50	11,530.00	6.06E-03	6.51E-03
11,530.00	14,032.00	5.42E-03	5.55E-03
14,032.00	17,511.50	4.92E-03	4.97E-03
17,511.50	100,000.00	3.88E-03	3.87E-03

Source: Output DTN: MO0308SPACO2GL.001.

Table 6.7-5. Lookup Tables for Total System Performance Assessment-License Application Analysis of In-Drift and Invert $p\text{CO}_2$ for W7 (CS500) Seepage Water

w7, CS500		Drift	Invert
Start (yr)	End (yr)	Partial Pressure $\text{CO}_{2(g)}$ bars	Partial Pressure $\text{CO}_{2(g)}$ bars
1.00	2.50	4.73E-03	5.11E-03
2.50	7.50	4.04E-03	4.22E-03
7.50	15.00	3.72E-03	3.88E-03
15.00	25.00	3.38E-03	3.34E-03
25.00	35.00	3.19E-03	3.20E-03
35.00	45.00	3.12E-03	3.28E-03
45.00	50.50	3.04E-03	3.16E-03
50.50	52.00	1.69E-03	5.02E-03
52.00	54.00	5.97E-04	2.49E-03
54.00	57.50	3.36E-04	1.43E-03
57.50	67.50	7.83E-05	4.08E-04
67.50	87.50	2.69E-04	3.49E-04
87.50	125.00	8.20E-04	9.42E-04
125.00	175.00	1.82E-03	1.92E-03
175.00	225.00	2.30E-03	2.36E-03
225.00	275.00	2.10E-03	2.12E-03
275.00	325.00	1.63E-03	1.64E-03
325.00	375.00	1.17E-03	1.16E-03
375.00	450.00	7.66E-04	7.63E-04
450.00	550.00	3.55E-04	3.37E-04
550.00	625.00	4.25E-04	3.97E-04
625.00	675.00	6.34E-04	5.70E-04
675.00	725.50	8.95E-04	8.25E-04
725.50	767.00	1.24E-03	1.17E-03
767.00	792.00	1.42E-03	1.39E-03
792.00	900.50	1.64E-03	1.57E-03
900.50	1,100.50	3.28E-03	3.26E-03
1,100.50	1,300.50	4.37E-03	4.38E-03
1,300.50	1,501.00	5.55E-03	5.50E-03
1,501.00	1,701.00	6.30E-03	6.32E-03
1,701.00	1,901.00	6.91E-03	6.87E-03
1,901.00	2,101.00	6.45E-03	6.05E-03
2,101.00	2,301.50	7.26E-03	9.04E-03
2,301.50	2,496.50	7.62E-03	9.86E-03
2,496.50	2,797.00	6.73E-03	1.75E-02
2,797.00	4,002.50	6.99E-03	1.51E-02
4,002.50	6,004.00	6.76E-03	8.96E-03
6,004.00	8,505.50	7.17E-03	8.26E-03
8,505.50	11,301.50	7.74E-03	8.14E-03
11,301.50	13,803.00	7.67E-03	7.96E-03
13,803.00	17,511.50	7.18E-03	7.26E-03
17,511.50	100,000.00	5.91E-03	5.79E-03

Source: Output DTN: MO0308SPACO2GL.001.

6.7.3 THC Seepage Water Equilibrium Gas Fugacity

EQ3 calculations are run to equilibrate and speciate the water compositions of the 11 bin waters abstracted in Section 6.6 (Table 6.6-5). The resulting water compositions and the corresponding gas fugacities are provided in Table 6.7-6. The fugacity at the wetting front, which is defined as the closest cell to the drift center that has saturation levels above zero (i.e., the calculation cell is not completely dried out).

The complete set of fugacity values from all 368 waters listed in Table 6.6-1 (rather than the subset presented in Table 6.7-6) can be extracted from the calculated EQ3 3o files archived in DTN: MO0303MWDSCMAB.000 using the GETEQDATA V1.0.1 1 (BSC 2003 [DIRS 161900]) data extraction tool. Values of gas fugacity as a function of time are available in the EQ6 output files listed in Table 6.6-1 and are archived in DTN: MO0303MWDEBSSM.000.

6.7.4 Dust Leachate Equilibrium Gas Fugacity

In conjunction with the aqueous chemical results produced in Section 6.10.6.4, equilibrium gas fugacity values are available for the six binned dust leachate water compositions selected to represent the range of leachate water chemistries (DTN: MO0310SPADLBU4.001, *6 bin EQ3 gas and dust leachate water extract.xls*). The values shown by the Table 6.7-7 graphical plots are representative of the equilibrium gas values at atmospheric $p\text{CO}_2$ ($10^{-3.5}$ bar), at or near ambient temperatures (25°C), and in equilibrium with solutions formed by dust deliquescence. For temperatures above this, the values that are found in the calculated EQ6 output files (Table 6.10-12) should be used.

Table 6.7-6. Equilibrium Gas Fugacity, Temperatures, pH, and Ionic Strengths from the 11 Bin Waters

	Bin01.3o	Bin02.3o	Bin03.3o	Bin04.3o	Bin05.3o	Bin06.3o	Bin07.3o	Bin08.3o	Bin09.3o	Bin10.3o	Bin11.3o
Temp (°C)	112	109	104	105	95.6	65.1	56.3	40.2	91.8	56.3	95.6
pH	7.41	7.58	7.62	7.9	7.63	7.7	7.75	7.94	8.14	7.82	7.76
I (molal)	4.93E-02	2.05E-02	9.74E-03	4.92E-03	1.13E-02	1.12E-02	1.24E-02	9.77E-03	5.10E-03	8.71E-03	7.06E-03
H ₂ O _(g) *	1.77E-01	1.34E-01	6.07E-02	7.56E-02	-6.92E-02	-6.02E-01	-7.77E-01	-1.13E+00	-1.30E-01	-7.77E-01	-6.91E-02
O _{2(g)} *	-7.00E-01	-7.00E-01	-7.00E-01	-7.00E-01	-7.00E-01	-7.00E-01	-7.00E-01	-7.00E-01	-7.00E-01	-7.00E-01	-7.00E-01
CO _{2(g)} *	-3.47E+00	-3.36E+00	-3.05E+00	-3.38E+00	-2.78E+00	-2.21E+00	-2.18E+00	-2.25E+00	-2.59E+00	-2.10E+00	-2.45E+00
HF _(g) *	-9.82E+00	-9.91E+00	-9.91E+00	-1.01E+01	-9.69E+00	-1.07E+01	-1.11E+01	-1.19E+01	-1.03E+01	-1.11E+01	-9.67E+00
HCl _(g) *	-1.23E+01	-1.32E+01	-1.35E+01	-1.43E+01	-1.38E+01	-1.49E+01	-1.53E+01	-1.69E+01	-1.51E+01	-1.61E+01	-1.43E+01
HNO _{3(g)} *	-1.38E+01	-1.44E+01	-1.51E+01	-1.55E+01	-1.53E+01	-1.67E+01	-1.70E+01	-1.82E+01	-1.57E+01	-1.75E+01	-1.56E+01
NO _{2(g)} *	-2.40E+01	-2.46E+01	-2.54E+01	-2.58E+01	-2.58E+01	-2.80E+01	-2.87E+01	-3.04E+01	-2.64E+01	-2.91E+01	-2.62E+01
H _{2(g)} *	-2.99E+01	-3.02E+01	-3.08E+01	-3.07E+01	-3.17E+01	-3.53E+01	-3.65E+01	-3.88E+01	-3.21E+01	-3.65E+01	-3.17E+01
N ₂ O _{5(g)} *	-3.28E+01	-3.40E+01	-3.53E+01	-3.61E+01	-3.57E+01	-3.84E+01	-3.92E+01	-4.16E+01	-3.66E+01	-4.01E+01	-3.64E+01

Source: Output DTN: MO0304SPAA11GC.000.

* Units are log fugacities in bars.

Table 6.7-7. Equilibrium Gas Fugacity, Temperatures, pH and Ionic Strengths from the 6 Bin Dust Leachate Waters

Filename	p25_25b.3o	p26_25b.3o	s80c25b.3o	s86a25b.3o	s90b25b.3o	s92a25b.3o
Temp (°C)	25	25	25	25	25	25
pH	8.54	8.40	8.54	8.23	8.09	8.05
aw	1.00	1.00	1.00	1.00	1.00	1.00
(I)	6.29E-03	3.80E-03	5.43E-03	2.01E-03	2.74E-03	1.15E-03
O _{2(g)}	-0.67	-0.67	-0.67	-0.67	-0.67	-0.67
H ₂ O _(g)	-1.50	-1.50	-1.50	-1.50	-1.50	-1.50
CO _{2(g)}	-3.50	-3.50	-3.50	-3.50	-3.50	-3.50
HF _(g)	-14.50	-14.11	-14.33	-14.30	-14.16	-13.99
HCl _(g)	-18.26	-18.29	-18.55	-18.42	-18.26	-18.23
HNO _{3(g)}	-18.31	-18.39	-18.34	-18.65	-18.34	-18.79
HBr _(g)	-22.23	-22.09	-22.74	-22.54	-21.98	-22.36
NO _{3(g)}	-30.99	-31.08	-31.02	-31.33	-31.02	-31.47
H _{2(g)}	-41.22	-41.22	-41.22	-41.22	-41.22	-41.22
N ₂ O _{5(g)}	-41.65	-41.83	-41.71	-42.34	-41.71	-42.61

Source: Output DTN: MO0310SPADLBU4.001.

NOTE: * Units are log fugacity in bars.

6.8 GROUND SUPPORT INTERACTIONS WITH SEEPAGE WATER

This section evaluates the impact on seepage water chemistry from interactions with prevalent components of the ground support system and invert and their corrosion products. The materials of interest have been tabulated in Table 4.1-22, and are comprised of carbon steels and Stainless Steel Type 316L (also see in-drift schematic Figure 6.4-1). Based upon the short lifetime estimates of carbon or low alloy steels in the humid environments expected after closure, on the order of 50 yrs/cm relative lifetime (Figure 6.4-3), any effects of carbon steel on seepage chemistry are short-lived and not to be further considered. Also, the carbon steels are all located in or on the invert below the waste package. In contrast, Stainless Steel Type 316L has a significantly longer lifetime (relative per-cm lifetime on the order of 5,000 years, Figure 6.4-3) and is located over the crown of the drift, and therefore its effects upon the seepage water composition are considered.

Specifically, the present design calls for using Stainless Steel Type 316L perforated sheets and rock bolts (BSC 2004 [DIRS 169058]; Table 4.1-22) for the drift ground support system. Therefore, the elemental components of this steel are discussed, and this material is examined in detail with respect to its corrosion/precipitation and subsequent effect upon seepage water chemistry. The results presented here show that the Stainless Steel Type 316L corrosion process—the release of aqueous species and formation of corrosion products—has only negligible effect on the composition of incoming seepage waters.

6.8.1 Corrosion Product Concepts

Corrosion of the ground support materials is modeled as occurring by direct oxygen and proton consumption and can be generalized in Equation 6.8-1:

If this process alone occurs, the pH in the aqueous phase must increase. However, the magnitude of this effect is dependent upon the disposition of the metal ion released. If the ion is highly soluble, then the oxidation reaction shown in Equation 6.8-1 will dominate, and the pH of the seepage water will rise. However, if it is of low solubility then the resulting precipitation reaction must be accounted for. Typically, this reaction involves the formation of a hydroxide or oxide (or combined oxy-hydroxide). A general metal hydroxide formation reaction can be represented as shown in Equation 6.8-2:

This has the effect of releasing as many hydrogen ions as were consumed during corrosion: thereby, negating any effect upon the water chemistry. This is also the general case for oxide formation, shown by Equation 6.8-3:

The following subsections will discuss the three primary metals comprising Stainless Steel Type 316L (Fe, Ni, and Cr), that account for greater than 90 percent of this alloy by weight.

6.8.1.1 Iron (Fe)

Iron in the natural environment exists in two oxidation states. Fe(II) is the soluble form, but is not stable under the redox conditions in the drift (i.e., consistently oxic PO_2 , Section 6.7). Fe(III) primarily forms insoluble oxides and oxyhydroxides (e.g., Fe_2O_3 and $FeOOH$ respectively); its solubility product ranges from 10^{-36} to 10^{-42} at 25°C and $\text{pH} > 3$ based on the Pitzer Thermodynamic Database (DTN: SN0302T0510102.002 [DIRS 162572]), and it is increasingly soluble with lower pH values (Pankow 1991 [DIRS 105952], p. 231).

Table 6.8-1 shows the typical oxidation-reduction reactions for iron aqueous species and minerals. The Eh-pH diagram for iron plotted in Figure 6.8-1 shows that Fe(III) oxyhydroxides are the stable phase at the relatively high oxidation potentials expected at Yucca Mountain. The stability of the various forms of iron hydroxides and oxyhydroxides increases from amorphous $Fe(OH)_3$ to goethite to hematite (Fe_2O_3) at 25°C (Stumm and Morgan 1981 [DIRS 100829], p. 434). However, predicting if goethite or hematite will be present in a given system is difficult, because geochemical conditions may favor nucleation and growth of one or the other phase, and because goethite may persist metastably for millions of years, as the conversion of goethite to hematite can be very slow (Krauskopf 1979 [DIRS 105909], p. 208). However, in soils, goethite

tends to form at low temperatures (in cool or temperate climate zones), at high H₂O activity, and with higher organic matter contents. The hematite-to-goethite ratio usually increases with increasing soil temperature (Schwertmann and Taylor 1995 [DIRS 105959], pp. 398 to 400). The pH also plays a role in the preferred formation of the two phases. Goethite is favored in soils with low pH (3 to 7), whereas hematite is favored above pH 7 (Schwertmann and Taylor 1995 [DIRS 105959], pp. 401 to 402). However, if a small amount of Ti is present (<0.05 mol fraction) in the solution, it inhibits hematite formation and favors the formation of goethite (Fitzpatrick et al. 1978 [DIRS 105795]).

Table 6.8-1. Typical Oxidation–Reduction Reactions and Potential Fe Minerals

Reaction	Oxidation State	Minerals Formed
$2\text{Fe}^{2+} + \frac{1}{2}\text{O}_2 + 2\text{H}_2\text{O} = \text{Fe}_2\text{O}_3 + 4\text{H}^+$ $\text{Fe}_3\text{O}_4 + 2\text{H}^+ = \text{Fe}_2\text{O}_3 + \text{Fe}^{2+} + \text{H}_2\text{O}$ $2\text{FeOOH} + 2\text{H}^+ + \frac{1}{2}\text{O}_2 = \text{Fe}_2\text{O}_3 + \text{Fe}^{2+} + 2\text{H}_2\text{O}$	3	<i>Hematite</i> ($\alpha\text{-Fe}_2\text{O}_3$)
$\text{Fe}^{2+} + \frac{1}{4}\text{O}_2 + \frac{3}{2}\text{H}_2\text{O} = \text{FeOOH} + 2\text{H}^+$ $\text{Fe}_3\text{O}_4 + \text{H}^+ + \frac{1}{2}\text{O}_2 = \text{Fe}_2\text{O}_3 + \text{FeOOH}$	3	<i>Goethite</i> ($\alpha\text{-FeOOH}$)
$3\text{Fe}^{2+} + \frac{1}{2}\text{O}_2 + 3\text{H}_2\text{O} = \text{Fe}_3\text{O}_4 + 6\text{H}^+$	2.67	<i>Magnetite</i> (Fe_3O_4)

Source: Designed for Fe minerals using Tebo et al. 1997 [DIRS 105960], Table 2, as an example.

Given the slow rate of hematite formation, its suppression by high humidity conditions, and the presence of large quantities of Ti, goethite is expected to be the prevalent iron corrosion species for the period of regulatory interest. However, it is important to note that there is only a difference of <0.5 log units between the solubility of goethite and hematite, so, for modeling purposes, the choice of mineral has little impact.

Other minerals that could potentially form, based on the geochemical system at Yucca Mountain, are Fe carbonates and Fe-rich silicates. Given the low-temperature conditions, a likely iron-rich silicate mineral that may form would be a type of smectite clay (nontronite).

Source: Brookins 1988 [DIRS 105092].

NOTE: Approximated activities for dissolved species are: $Fe = 10^{-6}$, $Si = 10^{-3}$, $C = 10^{-3}$. Goethite and magnetite are considered Fe(III) solid phases.

Figure 6.8-1. Eh-pH Diagram for Part of the System Fe-C-Si-O-H at 25°C

Source: Brookins 1988 [DIRS 105092].

NOTE: Estimated activity for Ni = 10^{-4} , 10^{-6} .

Figure 6.8-2. Eh-pH Diagram for Part of the System Ni-O-H at 25°C

6.8.1.2 Nickel (Ni)

Only Ni(II) occurs at ambient environmental conditions. The higher oxidation states occur rarely and, even in those cases, it is not clear whether it is the ligand rather than the metal atom that is oxidized (Cotton and Wilkinson 1988 [DIRS 105732], p. 741). No other oxidation state would be expected under repository environmental conditions once Ni is released by oxidation of the metal alloys.

Once the Ni is released into an aqueous environment under oxidizing conditions, nickel hydroxides $[\text{Ni}(\text{OH})_2]$ are stable in a pH range between 8 and 12 (Figure 6.8-2). Otherwise, either the Ni^{2+} ion or the HNiO_2^- ions are in solution, indicating that nickel is relatively soluble under neutral-acidic conditions and under relatively alkaline conditions (Garrels and Christ 1990 [DIRS 144877], pp. 244 to 245).

Nickel tends to substitute for iron and manganese in solid phases, and tends to be coprecipitated as $\text{Ni}(\text{OH})_2$ with both iron oxides and manganese oxides (Hem 1985 [DIRS 115670]; Hem et al. 1989 [DIRS 105854]). Nickel will also adsorb to clays, iron and manganese oxides, and organic matter (McLean and Bledsoe 1992 [DIRS 108954]).

6.8.1.3 Chromium (Cr)

Unless otherwise indicated, the source of the following summary was taken from *Natural Attenuation of Hexavalent Chromium in Ground Water and Soils* (Palmer and Puls 1994 [DIRS 108991]).

Chromium exists in oxidation states ranging from +6 to -2; however, only the +6 and the +3 oxidation states are commonly encountered in the environment (refer to Eh/pH diagram in Figure 6.8-3). Cr(VI) exists in solution as the monomeric ions H_2CrO_4^0 , HCrO_4^- (bichromate), and CrO_4^{2-} (chromate), or as the dimeric ion $\text{Cr}_2\text{O}_7^{2-}$ (dichromate). The relative concentration of each of these species depends on both the pH of the chromium-laden water and the total concentration of Cr(VI).

Significant concentrations of H_2CrO_4^0 only occur at $\text{pH} \leq 1$. Above pH 6.5, CrO_4^{2-} generally dominates. Below pH 6.5, HCrO_4^- dominates when the Cr(VI) concentrations are low ($<30\text{mM}$), but $\text{Cr}_2\text{O}_7^{2-}$ becomes significant when concentrations are greater than 1mM , and may even dominate when the total Cr(VI) concentrations are greater than 30mM .

In the Cr(III)- H_2O system, Cr(III) exists predominantly as Cr^{3+} below a pH of 3.5. With increasing pH, hydrolysis of Cr^{3+} yields $\text{Cr}(\text{OH})^{2+}$, $\text{Cr}(\text{OH})_2^+$, $\text{Cr}(\text{OH})_3^0$, and $\text{Cr}(\text{OH})_4^-$ (corresponding to the species Cr^{3+} , CrOH^{2+} , CrO^+ , $\text{HCrO}_2(\text{aq})$, and CrO_2^- , respectively, in *data0.R2.ymp*). From under slightly acidic through alkaline conditions, Cr(III) can precipitate as an amorphous chromium hydroxide. Amorphous $\text{Cr}(\text{OH})_3$ can crystallize to $\text{Cr}(\text{OH})_3 \cdot 3\text{H}_2\text{O}$ or Cr_2O_3 (eskolaite) depending upon conditions. In the presence of Fe(III), trivalent chromium can precipitate as a solid solution, $(\text{Fe}_x\text{Cr}_{1-x})(\text{OH})_3$, with a lower solubility (Sass and Rai 1987 [DIRS 105957], Figure 1). If the pH of the system is between 6 and 12, the aqueous solubility of Cr(III) should be less than $1 \mu\text{mole/l}$. In addition, when the pH of the groundwater is greater than 4, Cr(III) coprecipitates with the Fe(III) in a solid solution with the general composition

$\text{Cr}_x\text{Fe}_{1-x}(\text{OH})_3$ (Sass and Rai 1987 [DIRS 105957], pp. 2,228 to 2,229; Amonette and Rai 1990 [DIRS 105701]). This should limit the concentration of Cr(III) to less than 10^{-6} molar, in the pH range from 6 through 12.

Cr(VI) is a strong oxidant and is reduced in the presence of electron donors. A common electron donor that could be present in the repository is ferrous iron. This reaction is very fast on the time scales of interest for most environmental problems, with the reaction going to completion in about five minutes even in the presence of dissolved oxygen (Eary and Rai 1988 [DIRS 105784]). When the pH is greater than 10, the rate of oxidation for Fe(II) by dissolved oxygen will exceed the rate of oxidation by Cr(VI) (Eary and Rai 1988 [DIRS 105784]).

Efficient Cr(VI) reduction in the presence of stainless steel, iron oxides, iron-containing silicates, and organic matter has been observed in several experiments. The reduction of Cr(VI) in the presence of hematite (Fe_2O_3) was demonstrated by Eary and Rai (1989 [DIRS 105788]). They attribute the reduction to the presence of a small amount of an FeO component in the hematite. They also suggest that the reaction occurs in solution after the FeO component has been solubilized. Reduction by biotite occurs when potassium ions are released to solution and Fe^{3+} ions are adsorbed onto the surface of the biotite. Potassium ions are released to maintain charge balance in the biotite structure. Reduction seems to occur even in oxygenated solutions. Lastly, experiments by Smith and Purdy (1995 [DIRS 162976]) addressing corrosion of Stainless Steel Type 316L and chromium speciation state in their abstract that: "Oxidation of chromium(III) to chromium(VI) was negligible at room temperature and only became significant in hot concentrated nitric acid. The rate of reduction of chromium(VI) back to chromium(III) by reaction with stainless steel or oxalic acid was found to be much greater than the rate of the reverse oxidation reaction."

Humic and fulvic acids are often associated with reduction by organic matter. The rate of reduction of Cr(VI) by the humic and fulvic acids will decrease with increasing pH. It increases with increasing initial Cr(VI) concentration and increases as the concentration of soil humic substances increases. At neutral pH, complete reduction of Cr(VI) may take many weeks. Sedlak and Chan (1997 [DIRS 105964]) studied the reaction of Cr(VI) with Fe(II) with respect to temperature and pH and determined that the reduction of Cr(VI) occurred on the time scale of minutes to months in sediments, soils, and waters that contained ferrous iron. Similar type experiments conducted in NaCl, NaClO_4 , and seawater solutions showed a parabolic dependence on pH, and the influences of temperature, ionic strength, and reductant concentration showed various linearly dependent effects on reduction (Pettine et al. 1998 [DIRS 105955]). In low temperature soil environments that have been contaminated with chromate-laden solutions, $\text{KFe}_3(\text{CrO}_4)_2(\text{OH})_6$ has been shown to precipitate and can reduce the amount of Cr(VI) in groundwater (Baron and Palmer 1996 [DIRS 105730]). This mineral, analogous to the sulfate mineral jarosite, is stable in oxidizing environments between a pH of 2 and 6.

Oxidation of Cr(III) to Cr(VI) has been achieved in three ways. The first requires dissolved oxygen, the second requires either manganese dioxide (MnO_2) (Eary and Rai 1987 [DIRS 105780]) or manganite (MnOOH) (Johnson and Xyla 1991 [DIRS 105878]), and the third requires using hot concentrated nitric acid (Smith and Purdy 1995 [DIRS 162976]). Eary and Rai (1987 [DIRS 105780], p. 1,188) found that dissolved oxygen is not an especially effective or likely way to oxidize Cr(III). However, interaction with manganese dioxide has been

demonstrated to increase as pH decreases and the ratio of surface area to solution volume increases. Eary and Rai 1987 developed an empirical rate law for the oxidation of Cr(III) by β -MnO₂ (pyrolusite). For manganite, the rate law has been determined to be independent of pH and ionic strength; however, it proceeds slower in the presence of organic ligands (Johnson and Xyla 1991 [DIRS 105878]).

Sorption of Cr(VI) onto goethite has been demonstrated to be a surface complexation mechanism dependent on pH. However, on magnetite, the mechanism has been determined to be reductive precipitation onto Fe(II) surface sites (Deng et al. 1996 [DIRS 105778]). Competition between common anionic groundwater ions (CO_{2(g)}, H₄SiO₄, and SO₄²⁻) and the CrO₄²⁻ ion is known to occur, where the adsorption of CrO₄²⁻ onto amorphous iron oxides was suppressed between 50 to 80 percent (Zachara et al. 1987 [DIRS 105963]).

6.8.2 Definition of Base Case

Base Case for Stainless Steel Type 316L—This is defined by the following:

- Material (sheets and rock bolts of Stainless Steel Type 316L) and dimensions as defined in *D&E/PA/C IED Subsurface Facilities Committed Materials* (BSC 2004 [DIRS 169058]) and *Repository Design Project, Repository/PA IED Emplacement Drift Committed Materials (2)* (BSC 2003 [DIRS 164101], Table 3) (Table 4.1-22)
- “Bin 11” seepage water (abstracted in Section 6.6.6, results in output DTN: MO0304MWDSAB11.001) as it is the most likely water chemistry for this stainless steel corrosion period (51 to 5,000 years, Table 6.13-3)
- Oxidation corrosion products that include Fe(III) and Cr(III)
- Primary controlling mineral phases for stainless steel corrosion products: goethite and amorphous chromium hydroxide
- Temperature of 25°C and fugacity of CO₂ and O₂ at 10⁻³ and 10^{-0.7} bar, respectively
- Abstracted Stainless Steel Type 316L corrosion rates based on output DTN: MO0407SPAPCEML.005 (Section 6.8.3).

The “maximum of the means” corrosion value for Stainless Steel Type 316L (Table 6.4-18) is used as the “Mean” to represent a relatively fast corrosion rate. As these corrosion rates are, in most experiments, based on weight loss, they include the effects of localized corrosion (if any) that occur during the experiments.

Interaction with the abstracted Bin 11 seepage water is chosen because this is the most likely water chemistry to exist during the period over which corrosion of stainless steel ground supports will occur (51 to 5,000 years, Table 6.13-3), and accounts for three of the four seepage water compositions shown in Tables 6.6-8 through 6.6-12. Bin 7 seepage water was selected as a sensitivity case in Section 6.12.4.

An Fe(III) phase has been selected as a corrosion end product that may influence seepage water chemistry because Fe(III), as opposed to Fe(II), is the oxidation state that would form under the relatively oxidizing conditions (atmospheric O₂ concentrations leading to significant dissolved oxygen content) and mild pH ranges of the seepage waters. The plotted diagram of Figure 6.8-1 shows that in the pH range of 6 through 9, with an O₂-fixed Eh range of ~0.8 through ~0.6 volts, the Fe(III) species are dominant.

Selection of Cr(III) over that of the more soluble Cr(VI) species is based on experimentally observed corrosion products, and on the kinetics and conditions required to obtain the fully oxidized Cr(VI) state (Smith and Purdy 1995 [DIRS 162976]). Smith and Purdy's (1995 [DIRS 162976], Figure 6) examination of the actual chromium speciation as a result of corrosion of Stainless Steel Type 316L demonstrated a predominance of the less soluble Cr(III) species, except under the conditions of hot concentrated nitric acid (111°C and >7 molar HNO₃). Other groups performing oxidation experiments, conducted under more ambient conditions, examined the oxidation of Cr(III) to Cr(VI) by dissolved oxygen. The experiments of Eary and Rai (1987 [DIRS 105780], p. 1,188) were performed from pH 4.0 to 12.5 without the detection of Cr(VI) formation in 24 days. Additionally, observed disequilibrium of dissolved oxygen in water correspond to the much more rapidly reacting O₂-H₂O₂ couple (Langmuir 1997 [DIRS 100051], Figure 11.5). The Eh values for this couple in the pH range from 6 to 9 are in the range of ~0.6 down to ~0.4 volts, corresponding to the Cr(III) field of Figure 6.8-3. However, Cr(VI) is examined as a sensitivity case in Section 6.12.4.

Source: Ball and Nordstrom 1998 [DIRS 163015].

NOTE: Eh units in volts (V) not Eh/V as shown on the figure.

Figure 6.8-3. The pe-pH diagram for aqueous inorganic chromium hydrolysis species. Hatched area indicates predominance region for $\text{Cr}(\text{OH})_3(\text{s})$.

Chromium Solid and Aqueous Species— After determining that the most common aqueous chromium oxidation state will be Cr(III) (and not Cr(VI) (Section 6.8.1.3)), all Cr(VI) related species are suppressed in the EQ3/6 chemical model calculations. Detailed examination of the remaining Cr(III) aqueous species is performed with respect to the solubility controlling chromium phase.

Based on the review article by Ball and Nordstrom (1998 [DIRS 163015]) of the original work by Rai et al. (1987 [DIRS 163369]), the amorphous chromium hydroxide [$\text{Cr}(\text{OH})_3$] was selected as the solubility limiting phase for Cr(III). The solubility constant was taken from the report by Ball and Nordstrom (1998 [DIRS 163015], Table 8). This constant at 25°C is used as a modification to the *data0.ympr.R2* database (DTN: MO0302SPATHDYN.000 [DIRS 161756]).

In addition, Rai et al. (1987 [DIRS 163369], p. 345) reiterate a previous review of literature (Rai and Zachara 1984 [DIRS 107060]) concluding that the Cr(III) solubility-controlling solids are thought to be either $\text{Cr}(\text{OH})_3$ or Cr(III) coprecipitated with Fe oxides and hydroxides. This amorphous chromium phase end-member solubility represents a conservative upper solubility, as there exists a well-characterized solid solution of chromium(III)-iron(III) hydroxide with solubility decreasing as the iron content increases (Sass and Rai 1987 [DIRS 105957]).

Five aqueous species in the EQ3/6 data input files are suppressed from the *data0.ympr.R2* database (DTN: MO0302SPATHDYN.000 [DIRS 161756]) prior to finalizing the model runs: three have undesired oxidation states (+6 and +5) and the other two had recently been characterized as relatively unimportant polynuclear Cr(III) species (these aqueous suppressions are listed in Table 6.8-4). The polynuclear species in the *data0.ympr.R2* database (DTN: MO0302SPATHDYN.000 [DIRS 161756]) are derived from the thermodynamic data compiled by Baes and Mesmer (1976 [DIRS 157860]). More recent experimental analysis by Rai et al. (1987 [DIRS 163369]) have cast doubt upon the importance of these polynuclear Cr(III) species, which the thermodynamic data (Baes and Mesmer 1976 [DIRS 157860]) predicts as becoming the dominant aqueous species at $\text{pH} < 6$. This has the effect of raising the solubility of $\text{Cr}(\text{OH})_3$ "unrealistically high and is completely at odds with the long-known descriptive solubility of $\text{Cr}(\text{OH})_{3(s)}$ " (Rai et al. 1987 [DIRS 163369], p. 346).

The remaining Cr(III) aqueous species are based upon thermodynamic estimates by Shock et al. (1997 [DIRS 127953]), who based their estimations upon the enthalpy of Cr^{3+} determined by Dellen et al. (1976 [DIRS 151392]). Though differing in their water content from the comprehensive review speciation equations of Ball and Nordstrom (1998 [DIRS 163015], Table 10) (e.g., CrO^+ in the database and not $\text{Cr}(\text{OH})_2^+$), they are retained unaltered as they represent the same basic species and make no numerical difference in calculation of formation constants using them. With the remaining aqueous chromium(III) species and the solubility constant of amorphous chromium(III) hydroxide (Ball and Nordstrom 1998 [DIRS 163015], Table 8) that resulted from the experimental work by Rai et al. (1987 [DIRS 163369]), the solubility of the amorphous chromium(III) hydroxide is calculated as a function of pH (4 through 13). The results of these calculations are compared to the Rai et al. (1987 [DIRS 163369], Figure 2) results plotted in Figure 6.8-4.

In this comparison, the detection limit reported by Rai et al. probably overestimates solubility in the pH range of 6 through 11. Their raw data show measurements well below their detection limits with values approaching those of the calculations (e.g., $\sim 4 \times 10^{-9}$ molar aqueous Cr in the report by Rai et al. (1987 [DIRS 163369], Figure 2), compared to a calculated 3.6×10^{-9} mol/kg H_2O at $\text{pH} = 9$ shown in the Figure 6.8-4 plot. At these concentrations the solution density is very close to 1.0 gm/cm^3 , making molar (mol/liter) and molal (mol/kg H_2O) units virtually equivalent.

This favorable comparison provides an independent confirmation of the remaining unsuppressed chromium(III) aqueous species in the *data0.ympr.R2* database (DTN: MO0302SPATHDYN.000 [DIRS 161756]), which were derived from independent thermodynamic data sources, as they reproduce chromium(III) solubility based on the log K value of hydroxide ($\text{Cr}(\text{OH})_{3(\text{am})}$) obtained from Ball and Nordstrom 1998 [DIRS 163015] (derived from Rai et al. 1987 [DIRS 163369]).

Output DTN: SN0312T0510102.013.

NOTE: Blue diamonds with lines compared to the 3-species model of Rai et al. (1987 [DIRS 163369], Figure 2, solid black lines) with their detection limit shown by the red dashed line.

Figure 6.8-4. EQ3/6 Calculated Chromium Solubility in Equilibrium with $\text{Cr}(\text{OH})_3(\text{am})$

Limitations—The base case is limited to supporting calculations at 25°C, because the primary mineral phase that controls Cr(III) solubility, $\text{Cr}(\text{OH})_3$, has its solubility defined only at this temperature (Rai et al. 1987 [DIRS 163369]). Rai et al. (1987 [DIRS 163369], Figure 4) only show that at 90°C the solubility of the $\text{Cr}(\text{OH})_3$ solid decreases, lowering the concentration of aqueous Cr(III) species by about two orders of magnitude. A CO_2 fugacity of 10^{-3} bars was chosen to be consistent with the median value from the ranges used for in-drift seepage evaporation (Section 6.9). Other fugacity values of 10^{-2} and 10^{-4} bars are examined to evaluate model uncertainty in Section 6.12.4.

6.8.3 Modeling Stainless Steel Type 316L and Its Corrosion Rate

The development of the abstraction starts with a review of the standard specifications for Stainless Steel Type 316L, as determined by the American Society for Testing and Materials standard (ASTM A 240/A 240M-02a 2002 [DIRS 162720], Table 1). This specification establishes weight-percentage values or limits or ranges for the various compositional elements. When ranges are specified, mean values are used to calculate the balance of Fe as 65.5 percent by weight (DTN: SN0312T0510102.013, *DegradationMolality.xls*, sheet name: Composition). This compares to 17 percent Cr by weight, resulting in a molar ratio of Fe:Cr of 3.59:1.0 (DTN: SN0312T0510102.013 sheet: degradation) that is rounded off to 3.6:1.0 and implemented in the modified *Data0.YMP.R2* EQ3/6 database file (original database DTN: MO0302SPATHDYN.000 [DIRS 161756]) as an abstracted mineral species titled Stainless Steel Type 316L.

The abstracted stainless steel species, whose molecular formula is $\text{Fe}_{3.6}\text{Cr}_{1.0}$, is defined by the dissociation reaction:

The reaction is not shown as being reversible because stainless steel will never precipitate. This is achieved operationally by providing an arbitrarily large solubility $\log K$ value of 266. The database text that was inserted into *Data0.YMP.R2* is also in DTN: SN0312T0510102.013 (*Cr-database.zip*).

The corrosion rate of Stainless Steel Type 316L controls the quantity of corrosion product and the extent to which corrosion affects the crown seepage water chemistry. The corrosion rate was estimated by determining the mean quantity of Stainless Steel Type 316L ground support over a one square meter section of drift wall. This quantity includes the Stainless Steel Type 316L sheets and rock bolts (Bernold and Swellex brand, respectively) from *D&E/PA/C IED Subsurface Facilities Committed Materials* (BSC 2004 [DIRS 169058]). A step-function for the corrosion rate was used to approximate the transition from dry to wet drift-wall conditions, which is estimated to occur around 2,000 years after emplacement as shown by the THC model results (DTN: LB0302DSCPTHCS.002 [DIRS 161976]). Seepage amounts, represented directly by the infiltration rates, were also taken from the THC spreadsheets (DTN: LB0302DSCPTHCS.002 [DIRS 161976], from "notes" sheet).

The rate of corrosion during the hot, dry period (up to 2000 years after closure) was taken as $0.113 \mu\text{m/yr}$, from the "316L SS" "Steam and atmospheric" "Mean" rate contained in Table 6.4-18 (DTN: MO0407SPAPCEML.005). At 2,000 plus years, a larger "fresh/salt water" corrosion rate was applied. The corrosion rate selected for wet conditions was $1.9391 \mu\text{m/yr}$, listed under Material "316L SS," "fresh/salt water," in Table 6.4-18 (DTN: MO0407SPAPCEML.005). To obtain the quantity (moles) of corroded steel in one year, the calculation multiplies the surface area with the corrosion rate, factoring in the density of Stainless Steel Type 316L (ASTM 1999 [DIRS 103515]) and its compositional makeup (ASTM 2002 [DIRS 162720]). This mole quantity of iron and chromium, as the amount released by corrosion per year, is then combined with the percolation flux calculated by THC (DTN: LB0302DSCPTHCS.002 [DIRS 161976], Sheet "notes") to generate a final molal quantity for input into the EQ3/6 speciation calculations.

These spreadsheet calculations, which are included in *DegradationMolality.xls* (DTN: SN0312T0510102.013, *DegradationMolality.zip*), provide a value for the corrosion rate in moles per year per square meter of the Stainless Steel Type 316L ground support.

6.8.4 Seepage-Steel Interaction Modeling and Base-Case Limitations

Details of the abstraction model calculation runs and results are supplied in the following subsections, concluding with a discussion on the limitations of this base-case model.

6.8.4.1 EQ3/6 Model Runs

The abstracted model for stainless steel ground support interaction with seepage water consists of the following sequential EQ3/6 calculation runs:

1. Initial EQ3NR speciation of Bin 11 seepage water (output DTN: MO0304MWDSAB11.001, a product output of this model) with trace quantities of "Fe²⁺" (10⁻³⁰ molal) and "Cr³⁺" (10⁻²⁰ molal) added; output pickup file from this feeds into 2) and 3)
2. EQ6 evaporation to 98 percent relative humidity of the Bin 11 water for basis of comparison
3. EQ6 "titration" run dissolving abstracted Stainless Steel Type 316L mineral by corrosion quantity; output second half of pickup file from this feeds into 4)
4. EQ6 evaporation to 98 percent relative humidity of the steel corrosion product containing Bin 11 water.

The input and output files associated with these four EQ3/6 calculation runs are listed in Table 6.8-2 and are documented in the output DTN: SN0312T0510102.013.

Table 6.8-2. EQ3/6 Input/Output Files for Stainless Steel Type 316L Corrosion Abstraction Model

Run	Input File Names	Output File Names	Pickup File Names
1	<i>Bin11.3i</i>	<i>bin11.3o</i>	<i>bin11.3p</i>
2	<i>Bin11e.6i</i>	<i>bin11e.6o</i>	<i>bin11e.6p</i>
3	<i>SSbin11.6i</i>	<i>ssbin11.6o</i>	<i>ssbin11.6p</i>
4	<i>ssbin11e.6i</i>	<i>ssbin11e.6o</i>	—

Source: Output DTN: SN0312T0510102.013.

NOTE: These files are contained in *Base case.zip*.

6.8.4.2 Mineral and AqueousSuppressions

The mineral suppressions include those identified in Section 6.6.2.6.4 of *In-Drift Precipitates/Salts Analysis* (BSC 2004 [DIRS 169863]; Table 6.5-2) and the three minerals identified in Table 6.6-2 (Albite, K-feldspar, and Celadonite). Due to the presence of ferric and chromium species, additional suppressions are required for these abstracted model calculation runs, and more silica species are suppressed as they saturated before amorphous silica in these 25°C calculation runs. These extra mineral suppressions and the bases for their suppression are listed in Table 6.8-3.

Table 6.8-3. Additional EQ3/6 MineralSuppressions Included for Seepage Ground Support Interactions

Mineral	Formula	Criteria Selected	Rationale	References
Tridymite	SiO ₂	Criterion 2	Tridymite forms at temperatures from about 700°C to 1,470°C.	Deer et al. 1992 [DIRS 163286], p. 465
Chalcedony	SiO ₂	Criterion 6	Modeling choice uses amorphous silica to control the silica phase and provide adequate conservatism.	Table D-1
Coesite	SiO ₂	Criterion 2	Coesite is a high-pressure SiO ₂ phase (>35 kbar) that will not form at atmospheric pressures.	Deer et al. 1992 [DIRS 163286], p. 466
Cristobalite (beta)	SiO ₂	Criterion 2	Cristobalite forms at temperatures from 330°C to 440°C; beta quartz transforms into beta cristobalite at 1,027°C and above 650 bars.	Deer et al. 1992 [DIRS 163286], pp. 465 to 466
Hematite	Fe ₂ O ₃	Criterion 3	Over long time frames, hematite is more stable than goethite, and the temperatures in the drift are elevated enough to warrant the precipitation of hematite, however if small amounts of Ti are present in solution, hematite is inhibited and goethite forms. Therefore, due to the large amount of Ti being emplaced in the repository drift, hematite will be suppressed (see discussion in Section 6.8.1.1).	Stumm and Morgan 1981 [DIRS 100829], p. 434 Fitzpatrick et al. 1978 [DIRS 105795]
Eskolaite	Cr ₂ O ₃	Criterion 2	Eskolaite is a common chromium mineral that may precipitate from a cooling magma. Although details of its liquid precipitation curves are still emerging, present data shows that 0.5 to 1.0% by mass of eskolaite precipitates in the range from 1,000°C to 1,150°C, and it is likely to begin precipitation above 920°C at atmospheric pressures.	Perez et al. 2001 [DIRS 163030], p. 4-31 Hrma et al. 2001 [DIRS 163031], Table 3.14, p. 3.27
Chromite	FeCr ₂ O ₄	Criterion 2	Chromite is a spinel mineral that is one of the earliest minerals to form in a cooling magma. May also occur in some metamorphic rocks. It does not form from aqueous solutions near or below 100°C.	Frye 1981 [DIRS 161804], p. 581
Magnesiochromite	MgCr ₂ O ₄	Criterion 2	Magnesiochromite is a spinel mineral similar to chromite.	Frye 1981 [DIRS 161804], p. 581

NOTE: The criteria used to include suppression of a mineral are defined in Section 6.5.4.

In calculation run 2 (Table 6.8-2), the zeolite clinoptilolite-K (0.015 Fe content) is also suppressed, because trace amounts of Fe cause numerical EQ6 calculation run instabilities. This suppression is removed for calculation runs 3 and 4, and this zeolite is not seen to form.

The suppression of a set of aqueous species is also deemed necessary from these seepage-steel interaction run abstractions and is described in Table 6.8-4. Reasons for these suppressions range from incorrect oxidation states to overly stable polymeric aqueous species.

Table 6.8-4. Aqueous SpeciesSuppressions Included for Seepage Ground Support Interactions

EQ3/6 Aqueous Species	Formula	Criteria Selected	Rationale	Reference(s)
Chromate	CrO_4^{2-}	Criteria 3	Oxidation of the initial Cr(III) corrosion species to this Cr(VI) basis species is very slow in the absence of strong oxidizing agent or extreme temperature and pH conditions	Eary and Rai 1987 [DIRS 105780], p. 1188 Smith and Purdy 1995 [DIRS 162976], Abstract
CrO_3Cl^-	CrO_3Cl^-	Criteria 3	Cr(VI) species, see above	as above
CrO_4^{3-}	CrO_4^{3-}	Criteria 3	Metastable Cr(V) species, not observable under near-equilibrium conditions	Niki 1985 [DIRS 163728], p. 460
$\text{Cr}_2(\text{OH})_2^{4+}$	$\text{Cr}_2(\text{OH})_2^{4+}$	Criteria 3	Previous studies that determined the polymeric species used in the database are overly stable. "The polymeric species of Cr(III) are generally absent in solutions at room temperature"	Rai et al. 1987 [DIRS 163369], pp. 345 to 346
$\text{Cr}_3(\text{OH})_4^{5+}$	$\text{Cr}_3(\text{OH})_4^{5+}$	Criteria 3	as above	as above

6.8.4.3 Result of Introducing Stainless Steel Type 316L to Bin 11

The effect of dissolving the abstracted Stainless Steel Type 316L species into Bin 11 water is negligible. Bin 11 water, with and without the 4.7×10^{-3} moles of Stainless Steel Type 316L added, has only two differences in the water chemistries and then only at the 6th significant figure (ionic strength and C total molality). This is shown in *316SS-base.xls* (DTN: SN0312T0510102.013, in filename *Base case.zip*) under the heading "Dissolution of SS316L into Bin 11 water." The effect of Stainless Steel Type 316L dissolution in the Bin 11 crown seepage water is summarized in Table 6.8-5. Values in this table represent the values calculated with the Stainless Steel Type 316L dissolution, minus the values of pure Bin 11 seepage waters, as determined at 100 and 98 percent relative humidity. The largest differences are less than 0.1 percent.

The results of sensitivity analyses (Section 6.12.4.1) do not conflict, with the exception of the pH affecting case where Cr(VI) is allowed to form.

Table 6.8-5. Absolute (Percent Relative) Differences Due to Stainless Steel Type 316L Dissolution in Bin 11 Seepage Water at 100 and 98 Percent Relative Humidity

RH	ΔpH	$\Delta(\text{Ionic Strength})$	$\Delta(\text{Cl moles/kg H}_2\text{O})$	$\Delta(\text{Si moles/kg H}_2\text{O})$	$\Delta(\text{C moles/kg H}_2\text{O})$
100	0.0001	1.5E-6 (2E-2)	3.6E-7 (3E-2)	1.7E-8 (8E-4)	3.6E-7 (3E-2)
98	-0.0001	-3.9E-4 (-0.05)	-1.1E-4 (-0.06)	-2.5E-5 (-0.07)	-6.1E-5 (-0.05)

Source: Output DTN: SN0312T0510102.013 (*316SS-base.xls* within *Base case.zip*).

There are no significant differences in the amounts of the mineral phases that exist in Stainless Steel Type 316L interacted and pure Bin 11 water at either 100 or 98 percent relative humidity; those minerals are: fluorite, sepiolite and $\text{SiO}_{2(\text{am})}$. Goethite and $\text{Cr}(\text{OH})_{3(\text{am})}$ are found only in the Stainless Steel Type 316L interacted water. Several trace ($< 10^{-8}$ moles) solid species are found only in one or the other of the waters; these consist of nontronite (Ca and K derivatives), erionite, and stellerite.

6.8.4.4 Limitations to Base-Case Results

Though there are several limitations discussed below, none are likely to affect the results of this section so much as to change the conclusion that stainless steel corrosion does not impact water chemistry.

Usage of only iron and chromium is considered a valid surrogate representation of stainless steel (encompassing ~85 percent by weight of total stainless steel composition), but is nonetheless a limitation. The next most abundant element is nickel at ~12 percent by weight. As nickel is more soluble than iron(III) or chromium(III) in mildly acidic conditions, it may be expected to affect pH slightly. However, not accounting for the nickel species is conservative as its inclusion would result in slightly higher pH solutions that are less likely to induce localized corrosion on the waste package outer barrier (BSC 2004 [DIRS 169984], Figure 6-50). The higher pH results from the dissolution of metallic Ni to Ni^{2+} with consumption of H^+ during the corrosion process (see reaction in Equation 6.8-1) without the corresponding production of H^+ during Ni-hydroxide precipitation (Equation 6.8-2). Note as well that this is a self-limiting process; as one obtains higher Ni^{2+} aqueous species concentrations and higher pH, the solubility of Ni^{2+} decreases and more aqueous $\text{Ni}(\text{OH})_2$ and solid are formed.

The temperature of 25°C imposed by the Cr(III) solubility data is a limitation. Direct comparisons of the effect of the corrosion products on the seepage waters at operational temperatures are not possible. This is conservative because Rai et al. (1987 [DIRS 163369], Figure 4) show decreasing solubility with increasing temperatures.

The analysis run calculations are restricted to using the *data0.ympr2* (DTN: MO0302SPATHDYN.000 [DIRS 161756]) non-Pitzer database and the B-dot activity model. Available Pitzer interaction parameters for Cr(III) species are limited, and the available pool was not deemed reliable enough to be implemented at this time.

6.9 IN-DRIFT SEEPAGE EVAPORATION

In-drift water compositions resulting from heating and evaporation of seepage are calculated with the in-drift precipitates/salts (IDPS) model (BSC 2004 [DIRS 169863]). This model includes the chemical influence of the in-drift atmosphere. Calculated outputs from the IDPS model are abstracted in the form of lookup tables for use as inputs to TSPA-LA calculations.

6.9.1 Seepage Water Inputs

The 11 EQ3 input files associated with the EQ6 output files listed in Table 6.6-4 (archived in DTN: MO0303MWDSCMAB.000) were copied and renamed (Bin 01 through Bin 11), and three additional mineral suppression inputs are added (Table 6.6-2). These 11 EQ3 3i input files are

run and the results archived are available in DTN: MO0304MWDSAB11.001. Data from the 11 EQ3 3o output files are extracted using GETEQDATA V1.0.1 (BSC 2003 [DIRS 161900]) to produce *11 bin EQ3 gas and water extract.xls* (archived in DTN: MO0304SPAA11GC.000). This spreadsheet is then used to produce Tables 6.9-1 and 6.9-2. These tables represent the EQ3NR equilibration and charge balancing of the 11 chemistries listed on Table 6.6-5. EQ3NR is used only to equilibrate the solution with respect to all aqueous species. It does not equilibrate the solutions with respect to minerals and gases. Subsequent EQ6 calculation runs are used for mineral and gas-phase equilibration. Table 6.9-3 lists the species that are used to charge balance the 11 bin compositions. As noted in Section 6.6.3, charge balancing is done on the least affected species, consistent with Section 6.6.3.1 of *In-Drift Precipitates/Salts Model* (BSC 2004 [DIRS 169863]). Comparison of Table 6.9-1 with the inputs found on Table 6.6-5 show that performing a charge balance does not impact the concentration of the given ion in the starting water.

The EQ3NR input and output files for the median bin waters that define the starting compositions of the 11 incoming seepage waters (Table 6.6-5) are documented in DTN: MO0304MWDSAB11.001 and are listed in Table 6.9-4.

6.9.2 Temperature and Carbon Dioxide

Temperature and carbon dioxide fugacity are varied to capture their effects on the compositional evolution of the bin waters during evaporation. Three values are chosen for each parameter, as described in Section 6.7.2. For temperature, the values are 40°C, 70°C, and 100°C. The CO₂ fugacity values are 10⁻², 10⁻³, and 10⁻⁴ bar. Each temperature is run for each CO₂ fugacity, resulting in nine combinations for each bin water. The input values for temperature and CO₂ fugacity are defined in the EQ6 input files of the IDPS model. These input files are based on the EQ6 input file templates of DTN: MO0303MWDIOJ13.000 [DIRS 162841]. The EQ3NR pickup files identified in Table 6.9-4 provide the bottom halves of the input files.

Table 6.9-1. Total EQ3NR Equilibrated Aqueous Elemental Compositions for the 11 Bins

	Bin01.3o	Bin02.3o	Bin03.3o	Bin04.3o	Bin05.3o	Bin06.3o	Bin07.3o	Bin08.3o	Bin09.3o	Bin10.3o	Bin11.3o
Temp (°C)	112	109	104	105	95.6	65.1	56.3	40.2	91.8	56.3	95.6
pH	7.41	7.58	7.62	7.90	7.63	7.7	7.75	7.94	8.14	7.82	7.76
(I)	4.93E-02	2.05E-02	9.74E-03	4.92E-03	1.13E-02	1.12E-02	1.24E-02	9.77E-03	5.10E-03	8.71E-03	7.06E-03
Al	3.27E-08	7.08E-08	5.02E-08	9.97E-08	8.03E-10	5.36E-09	3.71E-09	1.50E-09	6.09E-08	4.03E-09	1.42E-09
C	5.57E-05	9.06E-05	1.95E-04	1.64E-04	4.18E-04	2.93E-03	4.15E-03	6.92E-03	2.04E-03	5.74E-03	1.13E-03
Ca	1.75E-02	6.48E-03	2.15E-03	1.09E-03	1.36E-03	4.20E-04	6.40E-04	5.73E-04	7.24E-05	3.52E-04	3.34E-04
Cl	2.01E-02	5.02E-03	3.35E-03	1.03E-03	3.28E-03	3.32E-03	3.33E-03	5.61E-04	7.34E-04	6.00E-04	1.30E-03
F	1.93E-04	2.46E-04	3.48E-04	4.28E-04	1.00E-03	8.26E-04	6.73E-04	6.43E-04	9.77E-04	8.61E-04	1.38E-03
K	8.68E-04	5.40E-04	5.00E-04	2.38E-04	8.68E-04	6.25E-04	5.37E-04	2.76E-04	5.02E-04	4.17E-04	7.50E-04
Mg	1.70E-05	2.95E-06	4.13E-06	5.75E-07	1.13E-05	4.82E-05	6.94E-05	8.51E-05	2.54E-07	4.31E-05	6.34E-06
N	1.30E-03	5.46E-04	1.83E-04	1.33E-04	2.22E-04	1.04E-04	1.05E-04	3.97E-05	3.10E-04	4.25E-05	1.26E-04
Na	3.89E-03	2.63E-03	2.67E-03	1.26E-03	5.46E-03	8.08E-03	8.75E-03	7.30E-03	4.27E-03	6.81E-03	4.72E-03
S	8.87E-03	4.89E-03	1.50E-03	5.88E-04	1.77E-03	1.21E-03	1.22E-03	3.55E-04	1.18E-04	3.80E-04	7.29E-04
Si	9.42E-03	7.42E-03	6.96E-03	7.38E-03	1.22E-02	2.90E-03	2.35E-03	1.79E-03	4.15E-03	2.47E-03	1.19E-02

Source: Output DTN: MO0304SPAA11GC.000.

NOTE: All units, except temperature and pH, are in mols/kg H₂O.

Table 6.9-2. EQ3NR Equilibrium Speciation of the 11 Bins

Species	Bin01.3o	Bin02.3o	Bin03.3o	Bin04.3o	Bin05.3o	Bin06.3o	Bin07.3o	Bin08.3o	Bin09.3o	Bin10.3o	Bin11.3o
Cl ⁻	2.01E-02	5.02E-03	3.35E-03	1.03E-03	3.28E-03	3.32E-03	3.33E-03	5.61E-04	7.34E-04	6.00E-04	1.30E-03
Ca ²⁺	1.33E-02	4.70E-03	1.79E-03	9.74E-04	1.12E-03	3.71E-04	5.68E-04	5.09E-04	6.02E-05	3.09E-04	2.88E-04
SiO _{2(aq)}	9.02E-03	7.02E-03	6.60E-03	6.70E-03	1.16E-02	2.80E-03	2.27E-03	1.73E-03	3.60E-03	2.38E-03	1.11E-02
SO ₄ ²⁻	4.66E-03	3.14E-03	1.16E-03	4.88E-04	1.55E-03	1.18E-03	1.19E-03	3.49E-04	1.17E-04	3.74E-04	6.98E-04
CaSO _{4(aq)}	4.21E-03	1.75E-03	3.35E-04	1.00E-04	2.22E-04	2.72E-05	3.16E-05	5.74E-06	1.12E-06	6.28E-06	3.11E-05
Na ⁺	3.89E-03	2.63E-03	2.67E-03	1.26E-03	5.46E-03	8.08E-03	8.75E-03	7.30E-03	4.27E-03	6.81E-03	4.72E-03
NO ₃ ⁻	1.30E-03	5.46E-04	1.83E-04	1.33E-04	2.22E-04	1.04E-04	1.05E-04	3.97E-05	3.10E-04	4.25E-05	1.26E-04
K ⁺	8.68E-04	5.40E-04	5.00E-04	2.38E-04	8.68E-04	6.25E-04	5.37E-04	2.76E-04	5.02E-04	4.17E-04	7.50E-04
HSiO ₃ ⁻	3.97E-04	3.95E-04	3.62E-04	6.82E-04	5.97E-04	1.01E-04	7.70E-05	6.18E-05	5.47E-04	9.28E-05	7.52E-04
F ⁻	1.93E-04	2.46E-04	3.48E-04	4.28E-04	9.99E-04	8.25E-04	6.72E-04	6.43E-04	9.76E-04	8.60E-04	1.38E-03
O _{2(aq)}	1.57E-04	1.57E-04	1.56E-04	1.56E-04	1.56E-04	1.67E-04	1.76E-04	2.03E-04	1.56E-04	1.76E-04	1.56E-04
HCO ₃ ⁻	3.92E-05	7.30E-05	1.71E-04	1.47E-04	3.82E-04	2.80E-03	3.97E-03	6.68E-03	1.97E-03	5.53E-03	1.07E-03
OH ⁻	2.93E-05	3.51E-05	3.05E-05	5.81E-05	2.28E-05	6.89E-06	4.88E-06	2.85E-06	6.08E-05	5.64E-06	3.00E-05
CaOH ⁺	2.75E-05	1.40E-05	4.88E-06	5.88E-06	1.75E-06	7.53E-08	6.23E-08	2.18E-08	2.64E-07	4.24E-08	6.48E-07
Mg ²⁺	1.68E-05	2.91E-06	4.06E-06	5.55E-07	1.11E-05	4.65E-05	6.64E-05	7.93E-05	2.32E-07	4.02E-05	6.11E-06
CaHCO ₃ ⁺	6.95E-06	5.43E-06	5.30E-06	2.83E-06	6.19E-06	9.87E-06	1.91E-05	2.68E-05	1.88E-06	1.56E-05	4.85E-06
CaCO _{3(aq)}	6.04E-06	7.42E-06	8.15E-06	8.66E-06	9.06E-06	1.17E-05	2.13E-05	3.16E-05	8.97E-06	2.10E-05	9.85E-06
CO _{2(aq)}	3.34E-06	4.37E-06	9.28E-06	4.37E-06	1.83E-05	9.30E-05	1.15E-04	1.32E-04	2.95E-05	1.39E-04	3.90E-05
CO ₃ ²⁻	2.05E-07	4.01E-07	8.72E-07	1.28E-06	2.02E-06	1.54E-05	2.34E-05	4.91E-05	2.96E-05	3.64E-05	7.02E-06
MgOH ⁺	1.42E-07	3.73E-08	5.41E-08	1.71E-08	9.05E-08	6.85E-08	5.89E-08	3.52E-08	5.92E-09	4.55E-08	7.49E-08
NaF _(aq)	1.21E-07	1.19E-07	1.80E-07	1.13E-07	9.46E-07	8.18E-07	6.45E-07	4.42E-07	7.52E-07	6.67E-07	1.19E-06
HSO ₄ ⁻	1.16E-07	6.44E-08	2.17E-08	5.46E-09	2.13E-08	5.27E-09	3.51E-09	4.22E-10	4.94E-10	9.90E-10	7.65E-09
H ⁺	4.94E-08	3.14E-08	2.72E-08	1.38E-08	2.67E-08	2.26E-08	2.02E-08	1.28E-08	7.93E-09	1.69E-08	1.93E-08
AlO ₂ ⁻	3.27E-08	7.08E-08	5.02E-08	9.97E-08	8.03E-10	5.36E-09	3.71E-09	1.50E-09	6.09E-08	4.03E-09	1.42E-09
MgHCO ₃ ⁺	7.58E-09	2.89E-09	1.13E-08	1.58E-09	5.73E-08	1.18E-06	2.12E-06	3.96E-06	7.27E-09	1.96E-06	1.00E-07
MgCO _{3(aq)}	1.49E-09	9.14E-10	4.16E-09	1.15E-09	2.13E-08	4.46E-07	8.15E-07	1.85E-06	9.03E-09	9.05E-07	5.15E-08
NO ₂ ⁻	5.53E-13	1.71E-13	3.68E-14	2.89E-14	2.13E-14	5.03E-16	1.94E-16	1.08E-17	2.08E-14	7.82E-17	1.20E-14

Table 6.9-2. EQ3NR Equilibrium Speciation of the 11 Bins (continued)

Species	Bin01.3o	Bin02.3o	Bin03.3o	Bin04.3o	Bin05.3o	Bin06.3o	Bin07.3o	Bin08.3o	Bin09.3o	Bin10.3o	Bin11.3o
AlO ⁺	5.40E-14	6.57E-14	5.22E-14	2.69E-14	1.33E-15	5.16E-14	5.58E-14	3.58E-14	1.23E-14	4.37E-14	1.29E-15
AlOH ²⁺	1.49E-17	1.07E-17	7.87E-18	1.85E-18	2.75E-19	3.24E-17	4.88E-17	4.71E-17	8.01E-19	3.06E-17	1.83E-19
Al ³⁺	1.93E-21	6.81E-22	4.43E-22	4.29E-23	2.41E-23	1.16E-20	2.63E-20	3.90E-20	2.11E-23	1.25E-20	1.05E-23
ClO ₄ ⁻	9.85E-24	2.13E-24	1.18E-24	3.73E-25	8.53E-25	2.63E-25	1.82E-25	1.48E-26	1.65E-25	3.27E-26	3.37E-25
H ₂ (aq)	9.65E-34	4.76E-34	1.43E-34	1.82E-34	1.75E-35	3.83E-39	2.56E-40	1.25E-42	6.56E-36	2.56E-40	1.75E-35
NH ₃ (aq)	1.44E-49	1.54E-50	8.51E-52	4.76E-52	4.72E-53	8.89E-59	1.56E-60	1.65E-64	5.05E-54	5.45E-61	2.03E-53
NH ₄ ⁺	1.05E-49	8.13E-51	4.86E-52	1.32E-52	3.89E-53	2.91E-58	7.48E-60	1.33E-63	1.48E-54	2.19E-60	1.21E-53

Source: Output DTN MO0304SPAA11GC.000.

NOTE: All units are in moles/kg H₂O.

Table 6.9-3. List of Species Used to Charge Balance the Individual Water Chemistries

Bin	Charge-Balanced Ion
Bin 1	Ca ²⁺
Bin 2	Ca ²⁺
Bin 3	Ca ²⁺
Bin 4	Ca ²⁺
Bin 5	Na ⁺
Bin 6	Na ⁺
Bin 7	Na ⁺
Bin 8	Na ⁺
Bin 9	Na ⁺
Bin 10	Na ⁺
Bin 11	Na ⁺

Source: Output DTN: MO0304MWDSAB11.001.

Table 6.9-4. EQ3NR Input/Output Files for TSPA-LA Abstraction

Bin	Input File Names	Output File Names	Pickup File Names
Bin 1	<i>bin01.3i</i>	<i>bin01.3o</i>	<i>bin01.3p</i>
Bin 2	<i>bin02.3i</i>	<i>bin02.3o</i>	<i>bin02.3p</i>
Bin 3	<i>bin03.3i</i>	<i>bin03.3o</i>	<i>bin03.3p</i>
Bin 4	<i>bin04.3i</i>	<i>bin04.3o</i>	<i>bin04.3p</i>
Bin 5	<i>bin05.3i</i>	<i>bin05.3o</i>	<i>bin05.3p</i>
Bin 6	<i>bin06.3i</i>	<i>bin06.3o</i>	<i>bin06.3p</i>
Bin 7	<i>bin07.3i</i>	<i>bin07.3o</i>	<i>bin07.3p</i>
Bin 8	<i>bin08.3i</i>	<i>bin08.3o</i>	<i>bin08.3p</i>
Bin 9	<i>bin09.3i</i>	<i>bin09.3o</i>	<i>bin09.3p</i>
Bin 10	<i>bin10.3i</i>	<i>bin10.3o</i>	<i>bin10.3p</i>
Bin 11	<i>bin11.3i</i>	<i>bin11.3o</i>	<i>bin11.3p</i>

Source: Output DTN: MO0304MWDSAB11.001.

To cover the range of expected in-drift relative humidity values, the bin waters are evaporated to a water activity of 0.65 and diluted by a factor of 100. The starting bin waters are sufficiently dilute that they represented solutions in equilibrium with relative humidity between 99.9 and 99.99 percent. Dilution of water vapor is simulated for potential relative humidity values higher than the equilibrium relative humidity values of the starting bin water. Thus, for each temperature and CO₂ fugacity combination, two EQ6 input files are generated, one for evaporation and one for dilution. The resulting EQ6 input and output data files for the bin waters are listed in Table 6.9-5 and documented in DTN: MO0304MWDEBSSA.000. The file nomenclature is ??c#t%\$.6i or 6o, where:

- “??” is the two-digit bin number (01, 02, etc.)
- “#” is 2, 3, or 4 for fugacity of CO₂ equal to 10⁻², 10⁻³, or 10⁻⁴ bar, respectively
- “%” is 4, 7, or 1 for temperature equal to 40°C, 70°C, or 100°C, respectively, and
- “\$” is “e” or “c” for evaporation or dilution.

For example, file *01c211c.6i* is the EQ6 input file for bin 1 dilution at 100°C and a fugacity of CO₂ of 10⁻² bar.

6.9.3 Lookup Tables

The abstracted results of the evaporation and dilution calculations that are provided as direct input into TSPA-LA calculations are summarized in a set of lookup tables documented in DTN: MO0304SPACSALT.000. These lookup tables, listed in Table 6.9-6, include stated boundary conditions, abstracted output, and results of supplemental calculations. Each evaporation or dilution lookup table corresponds to one of the IDPS model output files identified in Table 6.9-5. Each row in these tables provides output parameter values as the water incrementally evolves due to evaporation or dilution, given the defined boundary conditions. Each value is defined by a unique equilibrium relative humidity, concentration factor, and relative evaporation rate.

The general lookup table format and the calculations placed in the lookup tables are developed and described in *In-Drift Precipitates/Salts Model* (BSC 2004 [DIRS 169863], Sections 6.7.3 and 6.6.3.5). The first three columns of these tables are supplemental spreadsheet calculations for: concentration factor (*CF*), relative evaporation rate (*Qe/Qs*), and dilution factor (*DF*). The next column is the equilibrium *RH*, calculated by multiplying the activity of water (in column K) by 100 percent. The rest of the columns are filled using GETEQDATA software version 1.0.1 (BSC 2003 [DIRS 161900]). Columns E through H show reaction progress and the boundary conditions for the starting water (i.e., the temperature and the fugacities of oxygen and carbon dioxide). Columns I through X show reaction progress, pH, ionic strength, mass of H₂O in the reactor, and the total concentrations of the aqueous components. Columns Y through AL present reaction progress, mass of H₂O, and the concentrations of potential acid-neutralizing species. Finally, columns AM through BD show the amounts of minerals accumulated. This last section is not included in the dilution lookup tables though small amounts of minerals (e.g., calcite) may be present, because mineral outputs from the IDPS model are only needed from evaporation runs.

Table 6.9-5. EQ6 Input/Output Files for TSPA-LA Abstraction

Bin	Input File Names	Output File Names
1	01c2t1e.6i, 01c3t1e.6i, 01c4t1e.6i, 01c2t4e.6i, 01c3t4e.6i, 01c4t4e.6i, 01c2t7e.6i, 01c3t7e.6i, 01c4t7e.6i, 01c2t1c.6i, 01c3t1c.6i, 01c4t1c.6i, 01c2t4c.6i, 01c3t4c.6i, 01c4t4c.6i, 01c2t7c.6i, 01c3t7c.6i, 01c4t7c.6i	01c2t1e.6o, 01c3t1e.6o, 01c4t1e.6o, 01c2t4e.6o, 01c3t4e.6o, 01c4t4e.6o, 01c2t7e.6o, 01c3t7e.6o, 01c4t7e.6o, 01c2t1c.6o, 01c3t1c.6o, 01c4t1c.6o, 01c2t4c.6o, 01c3t4c.6o, 01c4t4c.6o, 01c2t7c.6o, 01c3t7c.6o, 01c4t7c.6o
2	02c2t1e.6i, 02c3t1e.6i, 02c4t1e.6i, 02c2t4e.6i, 02c3t4e.6i, 02c4t4e.6i, 02c2t7e.6i, 02c3t7e.6i, 02c4t7e.6i, 02c2t1c.6i, 02c3t1c.6i, 02c4t1c.6i, 02c2t4c.6i, 02c3t4c.6i, 02c4t4c.6i, 02c2t7c.6i, 02c3t7c.6i, 02c4t7c.6i	02c2t1e.6o, 02c3t1e.6o, 02c4t1e.6o, 02c2t4e.6o, 02c3t4e.6o, 02c4t4e.6o, 02c2t7e.6o, 02c3t7e.6o, 02c4t7e.6o, 02c2t1c.6o, 02c3t1c.6o, 02c4t1c.6o, 02c2t4c.6o, 02c3t4c.6o, 02c4t4c.6o, 02c2t7c.6o, 02c3t7c.6o, 02c4t7c.6o
3	03c2t1e.6i, 03c3t1e.6i, 03c4t1e.6i, 03c2t4e.6i, 03c3t4e.6i, 03c4t4e.6i, 03c2t7e.6i, 03c3t7e.6i, 03c4t7e.6i, 03c2t1c.6i, 03c3t1c.6i, 03c4t1c.6i, 03c2t4c.6i, 03c3t4c.6i, 03c4t4c.6i, 03c2t7c.6i, 03c3t7c.6i, 03c4t7c.6i	03c2t1e.6o, 03c3t1e.6o, 03c4t1e.6o, 03c2t4e.6o, 03c3t4e.6o, 03c4t4e.6o, 03c2t7e.6o, 03c3t7e.6o, 03c4t7e.6o, 03c2t1c.6o, 03c3t1c.6o, 03c4t1c.6o, 03c2t4c.6o, 03c3t4c.6o, 03c4t4c.6o, 03c2t7c.6o, 03c3t7c.6o, 03c4t7c.6o
4	04c2t1e.6i, 04c3t1e.6i, 04c4t1e.6i, 04c2t4e.6i, 04c3t4e.6i, 04c4t4e.6i, 04c2t7e.6i, 04c3t7e.6i, 04c4t7e.6i, 04c2t1c.6i, 04c3t1c.6i, 04c4t1c.6i, 04c2t4c.6i, 04c3t4c.6i, 04c4t4c.6i, 04c2t7c.6i, 04c3t7c.6i, 04c4t7c.6i	04c2t1e.6o, 04c3t1e.6o, 04c4t1e.6o, 04c2t4e.6o, 04c3t4e.6o, 04c4t4e.6o, 04c2t7e.6o, 04c3t7e.6o, 04c4t7e.6o, 04c2t1c.6o, 04c3t1c.6o, 04c4t1c.6o, 04c2t4c.6o, 04c3t4c.6o, 04c4t4c.6o, 04c2t7c.6o, 04c3t7c.6o, 04c4t7c.6o
5	05c2t1e.6i, 05c3t1e.6i, 05c4t1e.6i, 05c2t4e.6i, 05c3t4e.6i, 05c4t4e.6i, 05c2t7e.6i, 05c3t7e.6i, 05c4t7e.6i, 05c2t1c.6i, 05c3t1c.6i, 05c4t1c.6i, 05c2t4c.6i, 05c3t4c.6i, 05c4t4c.6i, 05c2t7c.6i, 05c3t7c.6i, 05c4t7c.6i	05c2t1e.6o, 05c3t1e.6o, 05c4t1e.6o, 05c2t4e.6o, 05c3t4e.6o, 05c4t4e.6o, 05c2t7e.6o, 05c3t7e.6o, 05c4t7e.6o, 05c2t1c.6o, 05c3t1c.6o, 05c4t1c.6o, 05c2t4c.6o, 05c3t4c.6o, 05c4t4c.6o, 05c2t7c.6o, 05c3t7c.6o, 05c4t7c.6o
6	06c2t1e.6i, 06c3t1e.6i, 06c4t1e.6i, 06c2t4e.6i, 06c3t4e.6i, 06c4t4e.6i, 06c2t7e.6i, 06c3t7e.6i, 06c4t7e.6i, 06c2t1c.6i, 06c3t1c.6i, 06c4t1c.6i, 06c2t4c.6i, 06c3t4c.6i, 06c4t4c.6i, 06c2t7c.6i, 06c3t7c.6i, 06c4t7c.6i	06c2t1e.6o, 06c3t1e.6o, 06c4t1e.6o, 06c2t4e.6o, 06c3t4e.6o, 06c4t4e.6o, 06c2t7e.6o, 06c3t7e.6o, 06c4t7e.6o, 06c2t1c.6o, 06c3t1c.6o, 06c4t1c.6o, 06c2t4c.6o, 06c3t4c.6o, 06c4t4c.6o, 06c2t7c.6o, 06c3t7c.6o, 06c4t7c.6o
7	07c2t1e.6i, 07c3t1e.6i, 07c4t1e.6i, 07c2t4e.6i, 07c3t4e.6i, 07c4t4e.6i, 07c2t7e.6i, 07c3t7e.6i, 07c4t7e.6i, 07c2t1c.6i, 07c3t1c.6i, 07c4t1c.6i, 07c2t4c.6i, 07c3t4c.6i, 07c4t4c.6i, 07c2t7c.6i, 07c3t7c.6i, 07c4t7c.6i	07c2t1e.6o, 07c3t1e.6o, 07c4t1e.6o, 07c2t4e.6o, 07c3t4e.6o, 07c4t4e.6o, 07c2t7e.6o, 07c3t7e.6o, 07c4t7e.6o, 07c2t1c.6o, 07c3t1c.6o, 07c4t1c.6o, 07c2t4c.6o, 07c3t4c.6o, 07c4t4c.6o, 07c2t7c.6o, 07c3t7c.6o, 07c4t7c.6o
8	08c2t1e.6i, 08c3t1e.6i, 08c4t1e.6i, 08c2t4e.6i, 08c3t4e.6i, 08c4t4e.6i, 08c2t7e.6i, 08c3t7e.6i, 08c4t7e.6i, 08c2t1c.6i, 08c3t1c.6i, 08c4t1c.6i, 08c2t4c.6i, 08c3t4c.6i, 08c4t4c.6i, 08c2t7c.6i, 08c3t7c.6i, 08c4t7c.6i	08c2t1e.6o, 08c3t1e.6o, 08c4t1e.6o, 08c2t4e.6o, 08c3t4e.6o, 08c4t4e.6o, 08c2t7e.6o, 08c3t7e.6o, 08c4t7e.6o, 08c2t1c.6o, 08c3t1c.6o, 08c4t1c.6o, 08c2t4c.6o, 08c3t4c.6o, 08c4t4c.6o, 08c2t7c.6o, 08c3t7c.6o, 08c4t7c.6o

Table 6.9-5. EQ6 Input/Output Files for TSPA-LA Abstraction (Continued)

Bin	Input File Names	Output File Names
9	09c2t1e.6i, 09c3t1e.6i, 09c4t1e.6i, 09c2t4e.6i, 09c3t4e.6i, 09c4t4e.6i, 09c2t7e.6i, 09c3t7e.6i, 09c4t7e.6i, 09c2t1c.6i, 09c3t1c.6i, 09c4t1c.6i, 09c2t4c.6i, 09c3t4c.6i, 09c4t4c.6i, 09c2t7c.6i, 09c3t7c.6i, 09c4t7c.6i	09c2t1e.6o, 09c3t1e.6o, 09c4t1e.6o, 09c2t4e.6o, 09c3t4e.6o, 09c4t4e.6o, 09c2t7e.6o, 09c3t7e.6o, 09c4t7e.6o, 09c2t1c.6o, 09c3t1c.6o, 09c4t1c.6o, 09c2t4c.6o, 09c3t4c.6o, 09c4t4c.6o, 09c2t7c.6o, 09c3t7c.6o, 09c4t7c.6o
10	10c2t1e.6i, 10c3t1e.6i, 10c4t1e.6i, 10c2t4e.6i, 10c3t4e.6i, 10c4t4e.6i, 10c2t7e.6i, 10c3t7e.6i, 10c4t7e.6i, 10c2t1c.6i, 10c3t1c.6i, 10c4t1c.6i, 10c2t4c.6i, 10c3t4c.6i, 10c4t4c.6i, 10c2t7c.6i, 10c3t7c.6i, 10c4t7c.6i	10c2t1e.6o, 10c3t1e.6o, 10c4t1e.6o, 10c2t4e.6o, 10c3t4e.6o, 10c4t4e.6o, 10c2t7e.6o, 10c3t7e.6o, 10c4t7e.6o, 10c2t1c.6o, 10c3t1c.6o, 10c4t1c.6o, 10c2t4c.6o, 10c3t4c.6o, 10c4t4c.6o, 10c2t7c.6o, 10c3t7c.6o, 10c4t7c.6o
11	11c2t1e.6i, 11c3t1e.6i, 11c4t1e.6i, 11c2t4e.6i, 11c3t4e.6i, 11c4t4e.6i, 11c2t7e.6i, 11c3t7e.6i, 11c4t7e.6i, 11c2t1c.6i, 11c3t1c.6i, 11c4t1c.6i, 11c2t4c.6i, 11c3t4c.6i, 11c4t4c.6i, 11c2t7c.6i, 11c3t7c.6i, 11c4t7c.6i	11c2t1e.6o, 11c3t1e.6o, 11c4t1e.6o, 11c2t4e.6o, 11c3t4e.6o, 11c4t4e.6o, 11c2t7e.6o, 11c3t7e.6o, 11c4t7e.6o, 11c2t1c.6o, 11c3t1c.6o, 11c4t1c.6o, 11c2t4c.6o, 11c3t4c.6o, 11c4t4c.6o, 11c2t7c.6o, 11c3t7c.6o, 11c4t7c.6o

Source: Output DTN: MO0304MWDEBSSA.000.

Table 6.9-6. Lookup Tables for TSPA-LA Abstraction

Bin	Evaporation Lookup Tables	Dilution Lookup Tables
1	01c2t1e.xls.xls, 01c3t1e.xls.xls, 01c4t1e.xls.xls, 01c2t4e.xls.xls, 01c3t4e.xls.xls, 01c4t4e.xls.xls, 01c2t7e.xls.xls, 01c3t7e.xls.xls, 01c4t7e.xls.xls	01c2t1c.xls.xls, 01c3t1c.xls.xls, 01c4t1c.xls.xls, 01c2t4c.xls.xls, 01c3t4c.xls.xls, 01c4t4c.xls.xls, 01c2t7c.xls.xls, 01c3t7c.xls.xls, 01c4t7c.xls.xls
2	02c2t1e.xls.xls, 02c3t1e.xls.xls, 02c4t1e.xls.xls, 02c2t4e.xls.xls, 02c3t4e.xls.xls, 02c4t4e.xls.xls, 02c2t7e.xls.xls, 02c3t7e.xls.xls, 02c4t7e.xls.xls	02c2t1c.xls.xls, 02c3t1c.xls.xls, 02c4t1c.xls.xls, 02c2t4c.xls.xls, 02c3t4c.xls.xls, 02c4t4c.xls.xls, 02c2t7c.xls.xls, 02c3t7c.xls.xls, 02c4t7c.xls.xls
3	03c2t1e.xls.xls, 03c3t1e.xls.xls, 03c4t1e.xls.xls, 03c2t4e.xls.xls, 03c3t4e.xls.xls, 03c4t4e.xls.xls, 03c2t7e.xls.xls, 03c3t7e.xls.xls, 03c4t7e.xls.xls	03c2t1c.xls.xls, 03c3t1c.xls.xls, 03c4t1c.xls.xls, 03c2t4c.xls.xls, 03c3t4c.xls.xls, 03c4t4c.xls.xls, 03c2t7c.xls.xls, 03c3t7c.xls.xls, 03c4t7c.xls.xls
4	04c2t1e.xls.xls, 04c3t1e.xls.xls, 04c4t1e.xls.xls, 04c2t4e.xls.xls, 04c3t4e.xls.xls, 04c4t4e.xls.xls, 04c2t7e.xls.xls, 04c3t7e.xls.xls, 04c4t7e.xls.xls	04c2t1c.xls.xls, 04c3t1c.xls.xls, 04c4t1c.xls.xls, 04c2t4c.xls.xls, 04c3t4c.xls.xls, 04c4t4c.xls.xls, 04c2t7c.xls.xls, 04c3t7c.xls.xls, 04c4t7c.xls.xls
5	05c2t1e.xls.xls, 05c3t1e.xls.xls, 05c4t1e.xls.xls, 05c2t4e.xls.xls, 05c3t4e.xls.xls, 05c4t4e.xls.xls, 05c2t7e.xls.xls, 05c3t7e.xls.xls, 05c4t7e.xls.xls	05c2t1c.xls.xls, 05c3t1c.xls.xls, 05c4t1c.xls.xls, 05c2t4c.xls.xls, 05c3t4c.xls.xls, 05c4t4c.xls.xls, 05c2t7c.xls.xls, 05c3t7c.xls.xls, 05c4t7c.xls.xls
6	06c2t1e.xls.xls, 06c3t1e.xls.xls, 06c4t1e.xls.xls, 06c2t4e.xls.xls, 06c3t4e.xls.xls, 06c4t4e.xls.xls, 06c2t7e.xls.xls, 06c3t7e.xls.xls, 06c4t7e.xls.xls	06c2t1c.xls.xls, 06c3t1c.xls.xls, 06c4t1c.xls.xls, 06c2t4c.xls.xls, 06c3t4c.xls.xls, 06c4t4c.xls.xls, 06c2t7c.xls.xls, 06c3t7c.xls.xls, 06c4t7c.xls.xls
7	07c2t1e.xls.xls, 07c3t1e.xls.xls, 07c4t1e.xls.xls, 07c2t4e.xls.xls, 07c3t4e.xls.xls, 07c4t4e.xls.xls, 07c2t7e.xls.xls, 07c3t7e.xls.xls, 07c4t7e.xls.xls	07c2t1c.xls.xls, 07c3t1c.xls.xls, 07c4t1c.xls.xls, 07c2t4c.xls.xls, 07c3t4c.xls.xls, 07c4t4c.xls.xls, 07c2t7c.xls.xls, 07c3t7c.xls.xls, 07c4t7c.xls.xls
8	08c2t1e.xls.xls, 08c3t1e.xls.xls, 08c4t1e.xls.xls, 08c2t4e.xls.xls, 08c3t4e.xls.xls, 08c4t4e.xls.xls, 08c2t7e.xls.xls, 08c3t7e.xls.xls, 08c4t7e.xls.xls	08c2t1c.xls.xls, 08c3t1c.xls.xls, 08c4t1c.xls.xls, 08c2t4c.xls.xls, 08c3t4c.xls.xls, 08c4t4c.xls.xls, 08c2t7c.xls.xls, 08c3t7c.xls.xls, 08c4t7c.xls.xls

Table 6.9-6. Lookup Tables for TSPA-LA Abstraction (Continued)

Bin	Evaporation Lookup Tables	Dilution Lookup Tables
9	09c2t1e.xls.xls, 09c3t1e.xls.xls, 09c4t1e.xls.xls, 09c2t4e.xls.xls, 09c3t4e.xls.xls, 09c4t4e.xls.xls, 09c2t7e.xls.xls, 09c3t7e.xls.xls, 09c4t7e.xls.xls	09c2t1c.xls.xls, 09c3t1c.xls.xls, 09c4t1c.xls.xls, 09c2t4c.xls.xls, 09c3t4c.xls.xls, 09c4t4c.xls.xls, 09c2t7c.xls.xls, 09c3t7c.xls.xls, 09c4t7c.xls.xls
10	10c2t1e.xls.xls, 10c3t1e.xls.xls, 10c4t1e.xls.xls, 10c2t4e.xls.xls, 10c3t4e.xls.xls, 10c4t4e.xls.xls, 10c2t7e.xls.xls, 10c3t7e.xls.xls, 10c4t7e.xls.xls	10c2t1c.xls.xls, 10c3t1c.xls.xls, 10c4t1c.xls.xls, 10c2t4c.xls.xls, 10c3t4c.xls.xls, 10c4t4c.xls.xls, 10c2t7c.xls.xls, 10c3t7c.xls.xls, 10c4t7c.xls.xls
11	11c2t1e.xls.xls, 11c3t1e.xls.xls, 11c4t1e.xls.xls, 11c2t4e.xls.xls, 11c3t4e.xls.xls, 11c4t4e.xls.xls, 11c2t7e.xls.xls, 11c3t7e.xls.xls, 11c4t7e.xls.xls	11c2t1c.xls.xls, 11c3t1c.xls.xls, 11c4t1c.xls.xls, 11c2t4c.xls.xls, 11c3t4c.xls.xls, 11c4t4c.xls.xls, 11c2t7c.xls.xls, 11c3t7c.xls.xls, 11c4t7c.xls.xls

Source: DTN: Output MO0304SPACSALT.000.

NOTE: TSPA-LA modelers should use DTN: MO0310SPAPCEGS.000 as the source for the lookup tables as discussed in Section 8.2.1. The filenames in DTN: MO0310SPAPCEGS.000 do not carry the extra ".xls."

The values in the lookup tables may be used to define response surfaces so that interpolations and extrapolations (CO_2 fugacity parameter only, Section 6.12.4.3) may be obtained for more precise input values not provided in the tables. Table 6.9-7 displays the maximum equilibrium relative humidity value in the evaporation lookup table for a given boundary condition at or below which the information remains valid. If the equilibrium relative humidity exceeds this maximum value, then the corresponding dilution lookup table is used instead.

Table 6.9-7. Relative Humidity Boundaries Between Evaporation and Dilution Lookup Tables

Bin	10 ⁻² CO ₂ Fugacity (bars)			10 ⁻³ CO ₂ Fugacity (bars)			10 ⁻⁴ CO ₂ Fugacity (bars)		
	40°C	70°C	100°C	40°C	70°C	100°C	40°C	70°C	100°C
1	99.916%	99.915%	99.921%	99.917%	99.915%	99.921%	99.917%	99.915%	99.921%
2	99.962%	99.960%	99.957%	99.963%	99.961%	99.958%	99.963%	99.960%	99.957%
3	99.975%	99.973%	99.969%	99.976%	99.973%	99.970%	99.976%	99.973%	99.970%
4	99.985%	99.982%	99.978%	99.985%	99.983%	99.979%	99.986%	99.982%	99.978%
5	99.970%	99.967%	99.964%	99.971%	99.968%	99.965%	99.971%	99.968%	99.964%
6	99.964%	99.965%	99.966%	99.966%	99.967%	99.968%	99.968%	99.969%	99.969%
7	99.962%	99.964%	99.966%	99.965%	99.966%	99.967%	99.967%	99.968%	99.968%
8	99.969%	99.971%	99.971%	99.971%	99.972%	99.973%	99.974%	99.975%	99.974%
9	99.977%	99.975%	99.976%	99.978%	99.977%	99.978%	99.978%	99.979%	99.979%
10	99.969%	99.970%	99.971%	99.971%	99.972%	99.973%	99.974%	99.975%	99.975%
11	99.976%	99.973%	99.969%	99.976%	99.973%	99.970%	99.976%	99.973%	99.969%

Source: Output DTN: MO0304SPACSALT.000, RH MAP.xls, Tab "Sheet 1."

6.9.4 Illustration of Results

Figures 6.9-1 through 6.9-6 graphically illustrate the results with plots of values from the *11c3t7e.xls.xls* lookup table. These are Bin 11 evaporation results at a temperature of 70°C and a CO₂ fugacity of 10⁻³ bar. Figures 6.9-1 and 6.9-2 plot the total elemental aqueous concentrations and pH as a function of relative humidity and concentration factor. Figures 6.9-3 and 6.9-4 plot the acid neutralizing capacity (ANC) (ANC in this case represents those species that contribute to or influence the pH) aqueous species concentrations and pH as a function of relative humidity and concentration factor. Figures 6.9-5 and 6.9-6 plot pH, the fixed CO₂ and O₂ fugacities, and the moles of minerals precipitated from one kilogram of incoming water as a function of relative humidity and concentration factor.

Results of the corresponding dilution lookup table (*11c3t7c.xls.xls*) are displayed in Figures 6.9-7 through 6.9-10. The first two figures show plots of the total elemental aqueous concentrations and pH as a function of relative humidity and dilution factor. The last two plot the ANC aqueous species concentrations and pH as a function of relative humidity and dilution factor. The results from the remainder of the lookup tables are provided in Appendix II.

Output DTN: MO0304SPACSALT.000.

Figure 6.9-1. Predicted Compositional Evolution as Bin 11 Waters Evaporate at 70°C and 10⁻³ CO₂ Fugacity, Plotted Versus Relative Humidity

Output DTN: MO0304SPACSALT.000.

Figure 6.9-2. Predicted Compositional Evolution as Bin 11 Waters Evaporate at 70°C and 10^{-3} CO_2 Fugacity, Plotted Versus Concentration Factor

Output DTN: MO0304SPACSALT.000.

Figure 6.9-3. The Predicted Concentrations of ANC Species During Evaporative Evolution of Bin 11 Water at 70°C and 10^{-3} Bar CO_2 Fugacity, Plotted Versus Relative Humidity

Output DTN: MO0304SPACSALT.000.

Figure 6.9-4. The Predicted Concentrations of ANC Species During Evaporative Evolution of Bin 11 Water at 70°C and 10^{-3} Bar CO_2 Fugacity, Plotted Versus Concentration Factor

Output DTN: MO0304SPACSALT.000.

Figure 6.9-5. Predicted Mineral Precipitation as Bin 11 Waters Evaporate at 70°C and 10^{-3} CO_2 Fugacity, Plotted Versus Relative Humidity

Output DTN: MO0304SPACSALT.000.

Figure 6.9-6. Predicted Mineral Precipitation as Bin 11 Waters Evaporate at 70°C and 10^{-3} CO_2 Fugacity, Plotted Versus Concentration Factor

Output DTN: MO0304SPACSALT.000.

Figure 6.9-7. Predicted Compositional Evolution as Bin 11 Waters are Diluted at 70°C and 10^{-3} CO_2 Fugacity, Plotted Versus Relative Humidity

Output DTN: MO0304SPACSALT.000.

Figure 6.9-8. Predicted Compositional Evolution as Bin 11 Waters are Diluted at 70°C and 10^{-3} CO_2 Fugacity, Plotted Versus Concentration Factor

Output DTN: MO0304SPACSALT.000.

Figure 6.9-9. The Predicted Concentrations of ANC Species During Dilution of Bin 11 Water at 70°C and 10^{-3} Bar CO_2 Fugacity, Plotted Versus Relative Humidity

Output DTN: MO0304SPACSALT.000.

Figure 6.9-10. The Predicted Concentrations of ANC Species During Dilution of Bin 11 Water at 70°C and 10^{-3} Bar CO_2 Fugacity, Plotted Versus Dilution Factor

6.10 IN-DRIFT DUST LEACHATE ANALYSES

This section presents the technical approach to evaluate dust deliquescence chemistry and construct a set of lookup tables for use in the TSPA-LA. Section 6.10.1 briefly discusses the physical processes that are evaluated, after which an assessment of the U.S. Geological Survey (USGS) ESF dust datasets is presented (Section 6.10.2). Finally, an evaluation of the dust leachate chemistry and its abstraction into lookup tables is performed (Sections 6.10.3 through 6.10.7). The lookup tables are constructed based on the EQ3/6 (v. 8.0) calculations using thermodynamic database *data0.yprf* (Section 4.1.4; DTN: SN0302T0510102.002 [DIRS 162572]) and the USGS data on dust leachate compositions (DTNs: MO0207EBSDUSTS.020 [DIRS 162556] and MO0209EBSDUST2.030 [DIRS 162557]). Figure 6.10-1 shows the flow of the dust leachate abstraction process as derived for implementation in the TSPA-LA.

Figure 6.10-1. Flow Chart Representing the Dust Leachate Analysis Abstraction Process

6.10.1 Conceptual Framework

Dust accumulated on waste packages or drift shields during the operational period may contain some components of soluble salts, which will cause water condensation if the in-drift humidity is higher than the minimum deliquescence point of the salts. The resulting concentrated solution can potentially affect the degradation of the engineered barriers. Based on chemical equilibrium, the activity of water in the condensed (or deliquesced) solution (a_w) is set equal to the RH in the drift.

Based on the conceptual framework outlined in Section 6.2, the chemistry of the condensed water is mainly controlled by the:

- Type and relative amounts of soluble salts present in the dust deposited on the waste packages or drip shields
- Relative humidity, temperature, and partial pressure of CO₂ in the drift.

The amount of water that is expected to be present upon deliquescence of the system eutectic mineral assemblage is extremely small (at best a few monolayers thick; see additional discussion on rock–water ratios in Section 6.11.3). Because of the randomness of the distribution of salt minerals within the dust, this water could be located anywhere in the dust and not in direct contact with the waste package. For TSPA-LA purposes the deliquesced water is modeled as

being directly in contact with the waste package surface. Section 6.11.3 discusses alternate conceptual models on salt and water distribution.

6.10.2 Evaluation of U.S. Geological Survey Datasets

The USGS has provided two sets of measurements on dust compositions, which constitute the basic input data for the dust deliquescence calculations (Section 4.1.6; DTNs: MO0207EBSDUSTS.020 [DIRS 162556] and MO0209EBSDUST2.030 [DIRS 162557]). The first set of measurements, presented in Table 4.1-19, was made on the samples collected throughout the ESF during site characterization activities. The second set of measurements, presented in Table 4.1-20, was made on samples sufficiently large for chemical analyses of size-classified aliquots. Three size distributions of dust samples were prepared for chemical analysis: 60 to 200 mesh, 200 to 325 mesh, and less than 325 mesh (Peterman et al. 2003 [DIRS 162819]).

Data used in the dust leachate analysis were collected in ESF several years after initial construction of the tunnel from June 2001 through September 2002. The following activities known to occur in the ESF could influence or alter the initial composition of dusts generated by the construction of potential emplacement drifts:

- Diesel emissions from trains
- Welding activities
- Conveyor belt operations
- Dust suppression activities
- Operation of construction equipment
- Drilling and blasting
- Accumulation of human and animal waste
- Ventilation dust.

Each of these activities could have significant impact on both local and repository wide dust compositions. In all cases, trace elements and organics are possible constituents in airborne particulates. The dust composition measurements indicate that a large portion of the dust in the ESF comes from rock crushing during tunnel construction. The mean SiO_2 , Al_2O_3 , Na_2O , and K_2O values for the size-classified dust fractions are within about 10 percent of the Topopah Spring Tuff (Ttp) rhyolite values of the crystal-poor member of the Topopah Spring Tuff (Ttp). The water-soluble anions and cations (Ca, Mg, Na, PO_4 , Na, Cl, Br, NO_3 , and SO_4) are progressively enriched in the finer fractions of the dust, indicating that these components could be derived from atmospheric aerosols or from salts formed by evaporation of construction water and native porewater. The presence of salts formed from construction water is indicated by low Cl/Br ratios, reflecting construction water tagging with a LiBr tracer (Peterman et al. 2003 [DIRS 162819]).

The variation in the compositions of dust samples collected and related leachates analyzed by the USGS (total of 59 leachate analyses) is used to represent their compositional variability within the repository (Assumption 5.2.1). Of the 59 measurements, two analyses (#00574984B and #00574984C in Table 4.1-20) were excluded from the dust deliquescence calculations because they were incomplete. Three more were excluded (#00574979A, #00574979B, and #00574979C) because they were not collected inside the ESF but at the surface near the north portal.

The concentrations of soluble constituents in the dust samples analyzed by the USGS (DTNs: MO0207EBSDUSTS.020 [DIRS 162556] and MO0209EBSDUST2.030 [DIRS 162557]) are expressed in concentration units of micrograms of species per gram of dust (referred as ppm units in the source DTN) (Peterman et al. 2003 [DIRS 162819]). In order to use this data in the EQ3/6 equilibrium and reaction path calculations, these values were recalculated as leachate solution compositions, with aqueous concentration units of micrograms of species per grams of H₂O. The conversion was done by dividing the values provided in the USGS DTNs by 20, which is the mass fraction factor (i.e., grams of H₂O/gram of dust) used in the dust leaching process. Conversions are given in DTN: SN0310T0510102.010 in *Table 4_dust_leachate_Conv.xls*.

6.10.3 Equilibrium of Dust Leachate Waters

Aqueous speciation calculations have been performed at 25°C with EQ3NR (BSC 2003 [DIRS 162228]) for 54 dust leachate samples. This set of calculations serves two purposes:

- Generating pickup files (*.3p) for subsequent evaporation calculations
- Selecting dust leachate samples for the evaporation calculations based on the calculated pH and the charge neutrality constraint.

The EQ3 input files (*.3i) used in the speciation calculations are generated according to the protocol outlined in *In-Drift Precipitates/Salts Model* (BSC 2004 [DIRS 169863]) using the EQ3/6 template files found in DTN: MO0303SPAMEQ36.000 [DIRS 162549].

Two deviations to the protocol outlined in the IDPS model are necessary due to the lack of direct pH or alkalinity measurements on dust leachate samples. First, pH is estimated by charge balancing on H⁺ ion and setting HCO₃⁻ concentration to be in heterogeneous equilibrium with a fixed CO_{2(g)} fugacity, as a strict charge neutrality constraint must be maintained to obtain physically meaningful results for the intended evaporation calculations. Then, based on the calculated pH values, samples with pH values outside the range of 4 to 10 are screened out. This is because the water-mineral interactions with finely comminuted rhyolitic rock, plus equilibria between in-drift solutions and gases at ambient temperatures, would buffer the leachate pH to within the range similar to that for seepage waters (pH = 7.4 to 8.1; Table 6.9-1). Moreover, underlying analytical uncertainties of the dust leachate solutions coupled with minor dust components not considered in the fluid analysis can account for charge imbalances in the computational evaluation of aqueous solution concentrations. Therefore, the pH range chosen for screening is broad compared to expected values, allowing as many samples as possible to span a wide chemical parameter space. The quantitative range of the charge imbalance cannot be

determined due lack of pH and HCO_3^- information; however, it seems to usually lie within a reasonable range (10 to 20 percent) because most of the resulting pH values are very reasonable. Based on the pH-screening criterion, two additional samples (#00574987A and #00574981A) have been excluded from the dust deliquescence calculations due to low pH, leaving 52 remaining samples.

The speciation calculations are performed at the temperature of 25°C, under the atmospheric CO_2 partial pressure ($10^{-3.5}$ bar) (Weast 1979 [DIRS 102865]) and with the suppression of the following minerals:

- Maximum microcline
- Dolomite
- Quartz
- Cristobalite (alpha)
- Glaserite
- Talc
- Magnesite
- All saponites.

The rationale and criteria for these mineral suppressions can be found on Table 6.5-2. These suppressions have also been documented in *In-Drift Precipitates/Salts Model* (BSC 2004 [DIRS 169863], Section 6.6.2.6.4). In addition to the mineral suppressions advanced by the IDPS model, several more suppressions are added. Three minerals (albite, K-feldspar, and celadonite) are suppressed for the reasons documented in Section 6.6.3 (Table 6.6-2). Two more minerals (cryolite and $\text{K}_2\text{Si}_4\text{O}_9$ [K-wadeite]) found precipitating in preliminary dust modeling are suppressed, and the rationale can be found in Table 6.10-1.

Table 6.10-2 lists the EQ3NR input files developed from the two original USGS dust leachate (DTNs: MO0207EBSDUSTS.020 [DIRS 162556] and MO0209EBSDUST2.030 [DIRS 162557]) after converting the leachable salt values to conventional aqueous concentration units (ppm) calculated in DTN: SN0310T0510102.010. The associated output and pickup files to these calculation runs are given in this table. The values listed on these two tables are shown in micrograms per gram of H_2O , or ppm. The values used in the input EQ3 files are entered as mg/L; thus, the density of the leachate solution was taken to be 1.0 kg/L. This simplification cannot significantly affect the results of the calculations since these are dilute solutions with solute fraction of less than 0.1 percent. These files are archived in DTN: SN0310T0510102.010.

Table 6.10-1. Rationale for the Suppression of Cryolite and K-Wadeite in Dust Leachate Model Analyses

Mineral	Formula	Criteria Selected	Rationale	References
Cryolite	Na_3AlF_6	Criterion 3	Associated with fluorite in pegmatite veins in granite and gneiss. This precipitation is normally at high temperatures and pressures.	Buhn and Rankin 1999 [DIRS 163753]
$\text{K}_2\text{Si}_4\text{O}_9$ (K-wadeite)	$\text{K}_2\text{Si}_4\text{O}_9$	Criterion 3	Appears to be a high-temperature, high-pressure mineral phase. The formation temperature for precipitation is about 770°C.	Kracek and Clark 1966 [DIRS 163754], Figure 13-7

6.10.4 Calculation of Mineralogy at Dryout

The dryout calculations are designed to obtain a general idea about the evolution of chemical composition of dust leachate samples at different degrees of evaporation. In these calculations, water was continuously removed from the system using the titration mode of the code EQ6 (BSC 2003 [DIRS 162228]). The dryout is defined as the titration point where less than $\sim 10^{-10}$ kg of water remain from the initial 1 kg of water. However, the amount of water left in the calculation when the eutectic point is reached is generally between 10^{-5} to 10^{-6} kg (Figures 6.13.18 to 6.13.22). This set of dryout calculations is performed at 25°C and atmospheric $p\text{CO}_2$. The EQ6 input files used in the dryout calculations are generated according to the protocol outlined in *In-Drift Precipitates/Salts Model* (BSC 2004 [DIRS 169863]), starting with the EQ6 evaporative template files found in DTN: MO0303SPAMEQ36.000 [DIRS 162549].

Temperature, pH, and aqueous concentrations of all dissolved components are copied from the EQ3NR pickup files (Table 6.10-2) and appended to the bottom half of the associated EQ6 input files. These EQ6 input files are then run and the resulting output file calculations are produced. These input and output files are listed on Table 6.10-3 and are archived in DTN: SN0310T0510102.010.

A Microsoft Excel spreadsheet (*Dust Leach End Salt Assem Rev 01.xls*, archived in DTN: MO0310SPADLBU4.001) is created using GETEQDATA Version 1.0.1 software (BSC 2003 [DIRS 161900]) by extracting data from the output files listed on Table 6.10-3. The endpoint equilibrium data listed in Table 6.10-4 are extracted, and within the spreadsheet, the Excel statistical tools are used to calculate the statistics found at the bottom of the table with results shown on Figure 6.10-2.

Table 6.10-2. EQ3NR Input/Output Files for Dust Leachate Analyses

Input Table	Field/Sample #	Input File Names	Output File Names	Pickup File Names
Table 4.1-19	SPC00573607	<i>p07_25b.3i,</i>	<i>p07_25b.3o,</i>	<i>p07_25b.3p,</i>
	SPC00573610	<i>p10_25b.3i,</i>	<i>p10_25b.3o,</i>	<i>p10_25b.3p,</i>
	SPC00573611	<i>p11_25b.3i,</i>	<i>p11_25b.3o,</i>	<i>p11_25b.3p,</i>
	SPC00573612	<i>p12_25b.3i,</i>	<i>p12_25b.3o,</i>	<i>p12_25b.3p,</i>
	SPC00573614	<i>p14_25b.3i,</i>	<i>p14_25b.3o,</i>	<i>p14_25b.3p,</i>
	SPC00573615	<i>p15_25b.3i,</i>	<i>p15_25b.3o,</i>	<i>p15_25b.3p,</i>
	SPC00573616	<i>p16_25b.3i,</i>	<i>p16_25b.3o,</i>	<i>p16_25b.3p,</i>
	SPC00573617	<i>p17_25b.3i,</i>	<i>p17_25b.3o,</i>	<i>p17_25b.3p,</i>
	SPC00573618	<i>p18_25b.3i,</i>	<i>p18_25b.3o,</i>	<i>p18_25b.3p,</i>
	SPC00573619	<i>p19_25b.3i,</i>	<i>p19_25b.3o,</i>	<i>p19_25b.3p,</i>
	SPC00573620	<i>p20_25b.3i,</i>	<i>p20_25b.3o,</i>	<i>p20_25b.3p,</i>
	SPC00573622	<i>p22_25b.3i,</i>	<i>p22_25b.3o,</i>	<i>p22_25b.3p,</i>
	SPC00573623	<i>p23_25b.3i,</i>	<i>p23_25b.3o,</i>	<i>p23_25b.3p,</i>
	SPC00573624	<i>p24_25b.3i,</i>	<i>p24_25b.3o,</i>	<i>p24_25b.3p,</i>
	SPC00573625	<i>p25_25b.3i,</i>	<i>p25_25b.3o,</i>	<i>p25_25b.3p,</i>
	SPC00573626	<i>p26_25b.3i,</i>	<i>p26_25b.3o,</i>	<i>p26_25b.3p,</i>
	SPC00573627	<i>p27_25b.3i,</i>	<i>p27_25b.3o,</i>	<i>p27_25b.3p,</i>
	SPC00573628	<i>p28_25b.3i,</i>	<i>p28_25b.3o,</i>	<i>p28_25b.3p,</i>
	SPC00573629	<i>p29_25b.3i,</i>	<i>p29_25b.3o,</i>	<i>p29_25b.3p,</i>
	SPC00573630	<i>p30_25b.3i,</i>	<i>p30_25b.3o,</i>	<i>p30_25b.3p,</i>
	SPC00573631	<i>p31_25b.3i,</i>	<i>p31_25b.3o,</i>	<i>p31_25b.3p,</i>
	SPC00573632	<i>p32_25b.3i,</i>	<i>p32_25b.3o,</i>	<i>p32_25b.3p,</i>
	SPC00573633	<i>p33_25b.3i,</i>	<i>p33_25b.3o,</i>	<i>p33_25b.3p,</i>
Table 4.1-20	00574979A	<i>s79a25b.3i,</i>	<i>s79a25b.3o,</i>	<i>s79a25b.3p,</i>
	00574979B	<i>s79b25b.3i,</i>	<i>s79b25b.3o,</i>	<i>s79b25b.3p,</i>
	00574979C	<i>s79c25b.3i,</i>	<i>s79c25b.3o,</i>	<i>s79c25b.3p,</i>
	00574980A	<i>s80a25b.3i,</i>	<i>s80a25b.3o,</i>	<i>s80a25b.3p,</i>
	00574980B	<i>s80b25b.3i,</i>	<i>s80b25b.3o,</i>	<i>s80b25b.3p,</i>
	00574980C	<i>s80c25b.3i,</i>	<i>s80c25b.3o,</i>	<i>s80c25b.3p,</i>
	00574981B	<i>s81b25b.3i,</i>	<i>s81b25b.3o,</i>	<i>s81b25b.3p,</i>
	00574981C	<i>s81c25b.3i,</i>	<i>s81c25b.3o,</i>	<i>s81c25b.3p,</i>
	00574982A	<i>s82a25b.3i,</i>	<i>s82a25b.3o,</i>	<i>s82a25b.3p,</i>
	00574982B	<i>s82b25b.3i,</i>	<i>s82b25b.3o,</i>	<i>s82b25b.3p,</i>
	00574982C	<i>s82c25b.3i,</i>	<i>s82c25b.3o,</i>	<i>s82c25b.3p,</i>
	00574983A	<i>s83a25b.3i,</i>	<i>s83a25b.3o,</i>	<i>s83a25b.3p,</i>
	00574983B	<i>s83b25b.3i,</i>	<i>s83b25b.3o,</i>	<i>s83b25b.3p,</i>
	00574983C	<i>s83c25b.3i,</i>	<i>s83c25b.3o,</i>	<i>s83c25b.3p,</i>
	00574984A	<i>s84a25b.3i,</i>	<i>s84a25b.3o,</i>	<i>s84a25b.3p,</i>
	00574985A	<i>s85a25b.3i,</i>	<i>s85a25b.3o,</i>	<i>s85a25b.3p,</i>
	00574985B	<i>s85b25b.3i,</i>	<i>s85b25b.3o,</i>	<i>s85b25b.3p,</i>
	00574985C	<i>s85c25b.3i,</i>	<i>s85c25b.3o,</i>	<i>s85c25b.3p,</i>
	00574986A	<i>s86a25b.3i,</i>	<i>s86a25b.3o,</i>	<i>s86a25b.3p,</i>
	00574986B	<i>s86b25b.3i,</i>	<i>s86b25b.3o,</i>	<i>s86b25b.3p,</i>
	00574986C	<i>s86c25b.3i,</i>	<i>s86c25b.3o,</i>	<i>s86c25b.3p,</i>
	00574987B	<i>s87b25b.3i,</i>	<i>s87b25b.3o,</i>	<i>s87b25b.3p,</i>
	00574987C	<i>s87c25b.3i,</i>	<i>s87c25b.3o,</i>	<i>s87c25b.3p,</i>
	00574990A	<i>s90a25b.3i,</i>	<i>s90a25b.3o,</i>	<i>s90a25b.3p,</i>
	00574990B	<i>s90b25b.3i,</i>	<i>s90b25b.3o,</i>	<i>s90b25b.3p,</i>
	00574990C	<i>s90c25b.3i,</i>	<i>s90c25b.3o,</i>	<i>s90c25b.3p,</i>
	00574991A	<i>s91a25b.3i,</i>	<i>s91a25b.3o,</i>	<i>s91a25b.3p,</i>
	00574991B	<i>s91b25b.3i,</i>	<i>s91b25b.3o,</i>	<i>s91b25b.3p,</i>
	00574991C	<i>s91c25b.3i,</i>	<i>s91c25b.3o,</i>	<i>s91c25b.3p,</i>
	00574992A	<i>s92a25b.3i,</i>	<i>s92a25b.3o,</i>	<i>s92a25b.3p,</i>
	00574992B	<i>s92b25b.3i,</i>	<i>s92b25b.3o,</i>	<i>s92b25b.3p,</i>
	00574992C	<i>s92c25b.3i,</i>	<i>s92c25b.3o,</i>	<i>s92c25b.3p,</i>

Source: Output DTN: SN0310T0510102.010, Directory EQ3_runs.

Table 6.10-3. EQ6 Input and Output Files Used for Determination of the Mineralogy at Dryout

EQ6 Input Files	EQ6 Output Files
p07_25b.6i, p10_25b.6i, p11_25b.6i, p12_25b.6i, p14_25b.6i, p15_25b.6i, p16_25b.6i, p17_25b.6i, p18_25b.6i, p19_25b.6i, p20_25b.6i, p22_25b.6i, p23_25b.6i, p24_25b.6i, p25_25b.6i, p26_25b.6i, p27_25b.6i, p28_25b.6i, p29_25b.6i, p30_25b.6i, p31_25b.6i, p32_25b.6i, p33_25b.6i, s79a25b.6i, s79b25b.6i, s79c25b.6i, s80a25b.6i, s80b25b.6i, s80c25b.6i, s81b25b.6i, s81c25b.6i, s82a25b.6i, s82b25b.6i, s82c25b.6i, s83a25b.6i, s83b25b.6i, s83c25b.6i, s84a25b.6i, s85a25b.6i, s85b25b.6i, s85c25b.6i, s86a25b.6i, s86b25b.6i, s86c25b.6i, s87b25b.6i, s87c25b.6i, s90a25b.6i, s90b25b.6i, s90c25b.6i, s91a25b.6i, s91b25b.6i, s91c25b.6i, s92a25b.6i, s92b25b.6i, s92c25b.6i	p07_25b.6o, p10_25b.6o, p11_25b.6o, p12_25b.6o, p14_25b.6o, p15_25b.6o, p16_25b.6o, p17_25b.6o, p18_25b.6o, p19_25b.6o, p20_25b.6o, p22_25b.6o, p23_25b.6o, p24_25b.6o, p25_25b.6o, p26_25b.6o, p27_25b.6o, p28_25b.6o, p29_25b.6o, p30_25b.6o, p31_25b.6o, p32_25b.6o, p33_25b.6o, s79a25b.6o, s79b25b.6o, s79c25b.6o, s80a25b.6o, s80b25b.6o, s80c25b.6o, s81b25b.6o, s81c25b.6o, s82a25b.6o, s82b25b.6o, s82c25b.6o, s83a25b.6o, s83b25b.6o, s83c25b.6o, s84a25b.6o, s85a25b.6o, s85b25b.6o, s85c25b.6o, s86a25b.6o, s86b25b.6o, s86c25b.6o, s87b25b.6o, s87c25b.6o, s90a25b.6o, s90b25b.6o, s90c25b.6o, s91a25b.6o, s91b25b.6o, s91c25b.6o, s92a25b.6o, s92b25b.6o, s92c25b.6o

Source: Output DTN: SN0310T0510102.010, Directory Evap.

Source: Output DTN: MO0310SPADLBU4.001

Figure 6.10-2. EQ6 Dust Leachate Water Mineralogy at the Dryout End Point at 25°C and Atmospheric $p\text{CO}_2$

6.10.5 Dust Leachate Abstraction

As discussed in Section 6.5, chemical equilibrium is the basis for determining the resulting chemistry of the dust deliquescence process. Figure 6.2-2 illustrates that the aqueous solutions formed by deliquescence of soluble minerals in dry dust are the same composition as those that result as the solutions are evaporated.

Table 6.10-4. EQ6 Dust Leachate Water pH, a_w , Ionic Strength (I) Cl, N, and Cl:N Ratios at the Dryout End Point at 25°C and Atmospheric $p\text{CO}_2$

Output Filename	pH	EQ6 End Point a_w	(I)	Cl Moles/ kg H ₂ O	N Moles/ kg H ₂ O	Cl/N Molal Ratio
p07_25b.6o	7.59	0.39	18.56	1.87	4.50	0.41
p10_25b.6o	8.45	0.60	11.53	2.64	2.33	1.13
p11_25b.6o	8.45	0.60	11.53	2.64	2.33	1.13
p12_25b.6o	8.44	0.60	11.54	2.51	2.41	1.04
p14_25b.6o	7.82	0.55	11.73	1.49	3.55	0.42
p15_25b.6o	8.44	0.60	11.54	2.51	2.41	1.04
p16_25b.6o	7.82	0.55	11.73	1.49	3.55	0.42
p17_25b.6o	7.82	0.55	11.73	1.49	3.55	0.42
p18_25b.6o	10.21	0.61	12.13	3.18	2.04	1.56
p19_25b.6o	8.44	0.60	11.54	2.51	2.41	1.04
p20_25b.6o	10.21	0.61	12.13	3.18	2.04	1.56
p22_25b.6o	7.82	0.55	11.73	1.49	3.54	0.42
p23_25b.6o	7.82	0.55	11.73	1.49	3.54	0.42
p24_25b.6o	10.20	0.60	11.96	2.46	2.44	1.01
p25_25b.6o	7.82	0.55	11.73	1.49	3.54	0.42
p26_25b.6o	8.44	0.60	11.54	2.51	2.41	1.04
p27_25b.6o	8.44	0.60	11.54	2.51	2.41	1.04
p28_25b.6o	7.82	0.55	11.73	1.49	3.54	0.42
p29_25b.6o	10.20	0.60	11.96	2.46	2.44	1.01
p30_25b.6o	8.44	0.60	11.54	2.51	2.41	1.04
p31_25b.6o	8.44	0.60	11.54	2.51	2.41	1.04
p32_25b.6o	8.45	0.60	11.53	2.64	2.33	1.13
p33_25b.6o	8.45	0.60	11.53	2.64	2.33	1.13
s80a25b.6o	8.63	0.61	11.67	3.25	2.04	1.60
s80b25b.6o	7.82	0.55	11.73	1.49	3.54	0.42
s80c25b.6o	7.64	0.35	17.09	2.35	2.12	1.11
s81b25b.6o	8.45	0.60	11.53	2.64	2.33	1.13
s81c25b.6o	7.78	0.50	14.82	5.67	4.64	1.22
s82a25b.6o	10.21	0.61	12.13	3.18	2.04	1.56
s82b25b.6o	8.44	0.60	11.54	2.51	2.41	1.04
s82c25b.6o	8.11	0.55	11.94	1.47	3.60	0.41
s83a25b.6o	10.21	0.61	12.13	3.18	2.04	1.56
s83b25b.6o	8.44	0.60	11.54	2.51	2.41	1.04
s83c25b.6o	7.82	0.55	11.73	1.49	3.54	0.42
s84a25b.6o	10.21	0.61	12.12	3.19	2.04	1.56

Table 6.10-4. EQ6 Dust Leachate Water pH, a_w , Ionic Strength (I) Cl, N, and Cl:N Ratios at the Dryout End Point at 25°C and Atmospheric $p\text{CO}_2$ (Continued)

Output Filename	pH	EQ6 End Point a_w	(I)	Cl Moles/ kg H ₂ O	N Moles/ kg H ₂ O	Cl/N Molal Ratio
s85a25b.6o	8.45	0.60	11.53	2.64	2.33	1.13
s85b25b.6o	8.45	0.60	11.53	2.64	2.33	1.13
s85c25b.6o	8.44	0.60	11.54	2.51	2.41	1.04
s86a25b.6o	10.21	0.61	12.12	3.18	2.04	1.56
s86b25b.6o	8.45	0.60	11.53	2.64	2.33	1.13
s86c25b.6o	7.82	0.55	11.74	1.49	3.55	0.42
s87b25b.6o	7.82	0.55	11.73	1.49	3.54	0.42
s87c25b.6o	7.82	0.55	11.73	1.49	3.54	0.42
s90a25b.6o	8.45	0.60	11.53	2.64	2.33	1.13
s90b25b.6o	7.81	0.61	10.43	2.77	2.15	1.29
s90c25b.6o	8.45	0.60	11.53	2.64	2.33	1.13
s91a25b.6o	7.82	0.61	10.42	2.80	2.14	1.31
s91b25b.6o	7.81	0.61	10.43	2.77	2.15	1.29
s91c25b.6o	8.45	0.60	11.53	2.64	2.33	1.13
s92a25b.6o	10.20	0.62	11.61	3.71	1.79	2.07
s92b25b.6o	10.21	0.61	12.12	3.19	2.04	1.04
s92c25b.6o	8.634	0.61	11.67	3.26	2.04	0.41
Mean	8.56	0.58	11.93	2.48	2.67	0.99
Min	7.59	0.35	10.42	1.47	1.79	0.41
Max	10.21	0.62	18.56	5.67	4.64	2.07
S	0.86	0.05	1.33	0.77	0.70	0.42
2S	1.73	0.10	2.66	1.54	1.39	0.84

Source: Output DTN: MO0310SPADLBU4.001, *Dust Leach End Salt Assem Rev 01.xls*, Tab "Data and Plots."

At equilibrium, deliquescence is reversible, and the reverse process is evaporation as defined in the considered conceptual model. The model results in the most highly deliquescent assemblage salts possible, this is unlikely to be the actual assemblages found in dry dust. The abstraction process and steps for dust deliquescence are similar to those used for in-drift seepage evaporation treated in Section 6.9. The selection of 52 dust leachate water compositions to be used to represent dust deliquescence was described in Section 6.10.3. Four steps are then followed to abstract water compositions potentially forming by deliquescence:

- Step 1: Use *In-Drift Precipitates/Salts Model* (BSC 2004 [DIRS 169863]) to calculate compositions that result from evaporating the dust leachate compositions to a common water activity equal to 0.65. This step characterizes the leachates by the chemical divides that the waters pass through as they are concentrated by evaporation. For convenience, the evaporated leachate compositions at a water activity equal to 0.65 are referred to as normalized compositions (Section 6.10.5.1).
- Step 2: Sort the normalized leachate compositions from Step 1 into groups that exhibit similar chemical characteristics. The chemical criteria used to sort the waters are

discussed in Section 6.10.5.2. Then, the corresponding original leachate compositions from Section 6.10.3 that serve as precursors to the normalized seepage water compositions are placed into a bin. This process is repeated for all normalized leachate groups. The result is a set of leachate composition bins, each populated with compositions that yield chemically similar solutions after they are concentrated by evaporation (Section 6.10.5.2).

- Step 3: Identify a representative water for each bin, as close to the statistical median as possible, and use it as an approximation of all the leachate compositions in the bin (Section 6.10.5.3.1).
- Step 4: Generate the probability distribution of the leachate compositions by determining the number of waters in each bin (Section 6.10.5.3.2).

The six median water compositions chosen using the above procedure are used as inputs to the IDPS model to generate lookup tables for water compositions produced by dust deliquescence for use in the TSPA-LA calculations.

6.10.5.1 Normalization of the Leachate Compositions

The compositions of dust leachates vary among different dust samples not only in terms of the molar ratios of the dissolved constituents, but also in terms of the absolute concentrations of these constituents. To group these waters into bins containing more or less homogeneous water types, these waters had to be normalized to reflect the compositions of water types at a common ionic strength or degree of concentration.

The method chosen to normalize these water compositions is identical to the method discussed in Section 6.6.3 and involves using *In-Drift Precipitates/Salts Model* (BSC 2004 [DIRS 169863]) to evaporate the dust leachate waters to a common activity of water. This approach accounts for the effects of nearly every chemical divide important to a particular water. Other methods, such as dividing each concentration by the ionic strength, cannot as accurately reveal the likely brine endpoint for a given water. It is important to capture the likely evaporative evolution pathways in the binning analysis, because brine types can influence waste package and drip shield corrosion rates.

As determined by the IDPS model evaporations reported in Section 6.10.4, the waters evaporatively evolve to several different brine types, most commonly nitrate brines, chloride brines, and their combinations. An activity of water (a_w) of 0.65 is chosen as the common end-point of these normalizing evaporation run calculations, because this is approximately the lowest value at which all calculation runs are above the deliquescence point. Also, the trend in solution constituent concentrations given by the extent of evaporation delineated up to this a_w value seems to define the predominant brine type expected with further evaporation. Therefore, a higher value of water activity is not chosen because the objective of the binning analysis is to classify the waters by the type of brine they will produce.

The same EQ6 input files as those for the dryout calculations in Section 6.10.4 (Table 6.10-3) are used for the normalization calculations as well. The only difference from the model protocol is

that the input files are modified so that the evaporations are stopped when the activity of water attains the value of 0.65. Therefore, refer to Table 6.10-3 for the list of input and output files generated for use in EQ6. These specific 65 percent evaporation files are found in output DTN: SN0310T0510102.010, in subdirectory 65RH.

6.10.5.2 Bin Generation

Binning the leachate compositions is accomplished by sorting compositions into groups, such that all compositions in a group yield chemically similar solutions after they are concentrated by evaporation. Four properties are identified as criteria for determining chemical similarity. They are defined in such a way that they yield relatively low intrabin compositional ranges, compared with the compositional range of all the waters. Choices of the chemical characteristics are treated later in this section.

First, normalized leachate compositions from Step 1 are sorted into groups that exhibited similar chemical characteristics. Then each of the original leachate compositions from Section 6.10.3 that is a precursor to each of the normalized leachate compositions in a particular group is placed into a single bin; this process was repeated for all of the normalized leachate groups. The result is a set of leachate composition bins, each populated with compositions that yielded chemically similar solutions after they concentrated by evaporation.

The final equilibration results from each output file, archived in DTN: SN0310T0510102.010 (subdirectory 65RH), have been extracted and tabulated in a single Excel spreadsheet using the GETEQDATA Version 1.0.1 (BSC 2003 [DIRS 161900]) software. This spreadsheet, *EBS Dust Leachate Binning Abstraction Rev 01.xls*, is archived in DTN: MO0310SPADLBU4.001.

The variables selected for extraction include pH, activity of water ($a_w \approx 0.65$), ionic strength (I), total molality of the aqueous constituents, and the log value of the cumulative number of moles of each mineral precipitated. Formulas were added to calculate various molar ratios and pH, and several graphs are inserted to illustrate the variability of these compositional parameters among different leachate samples (Figures 6.10-3 to 6.10-6). This set of information was needed before the waters can be grouped by similarity. Figures 6.10-3 through 6.10-6 are meant only to illustrate the general variation in results among dust leachate evaporations. The spreadsheet provides the actual values.

Grouping (or binning) of the normalized leachate waters is accomplished by sorting the waters by predominant traits. These four criteria resulted in the creation of six bins such that the compositional variation within each group is small compared to the variation between groups.

Source: Output DTN: MO0310SPADLBU4.001

Figure 6.10-3. Total Elemental Molalities and pH of All Waters Used in the Binning Analysis After Evaporation to 65 Percent Relative Humidity

Source: Output DTN: MO0310SPADLBU4.001

Figure 6.10-4. Molar Ratios in Brines After Evaporation to 65 Percent Relative Humidity (Plot 1)

Source: Output DTN: MO0310SPADLBU4.001.

Figure 6.10-5. Molar Ratios in Brines After Evaporation to 65 Percent Relative Humidity (Plot 2)

Source: Output DTN: MO0310SPADLBU4.001.

Figure 6.10-6. Mineral Assemblages After Evaporation to 65 Percent Relative Humidity

The evaporated waters are binned based on the following four criteria:

- Total aqueous Ca molality > 0.01 molal?
  - If yes, the water likely evaporates towards the calcium side of the calcite and gypsum chemical divides, resulting in brine that is depleted of carbonate and sulfate. These brines also tend to have neutral to acidic pH and very low fluoride concentrations due to the low solubility of fluorite (CaF_2). This criterion is identical to one used in the THC seepage abstraction in Section 6.6.4.
- Total aqueous CO_3 molality < 0.1 molal?
  - If yes, Ca is likely depleted by the precipitation of calcite. In some cases, Ca and CO_3 have low concentrations, so this criterion further divides the low Ca case above. Waters having low concentrations of both of these components tend to maintain a neutral pH as they evaporate. This criterion is identical to one used in the THC seepage abstraction in Section 6.6.4.
- Total aqueous Br molality > 2 molal?
  - This criterion segregates bin 2 from the other bins (Table 6.10-5), thus reducing intra-bin variability.
- Total aqueous SO_4 molality > 0.8 molal?
  - This criterion distinguishes waters in bin 6 from bin 5 and waters in bin 3 from bin 4 (Table 6.10-5), reducing intrabin variability. This criterion is identical to one used in the THC seepage abstraction in Section 6.6.4.

Table 6.10-5. Binning Criteria Answer Key

Bin	Ca > 0.01 Molal	Br > 2 molal	CO_3 < 0.1 molal	SO_4 > 0.8 molal
Bin 1	yes	no	yes	no
Bin 2	no	yes	yes	no
Bin 3	no	no	no	yes
Bin 4	no	no	no	no
Bin 5	no	no	yes	yes
Bin 6	no	no	yes	no

Source: Output DTN: MO0310SPADLBU4.001, *EBS Dust Leachate Binning Abstraction Rev 01.xls*, Tab "Abstraction Notes."

Columns containing "if/then/else" Excel-type commands are added to the spreadsheet to facilitate responding to each grouping criterion for each water. Waters having identical answers to the questions listed on Table 6.10-5 are placed in the same bin. Results are provided and plotted in *EBS Dust Leachate Binning Abstraction Rev 01.xls* spreadsheet (DTN: MO0310SPADLBU4.001). They are also shown in Figures 6.10-7 through 6.10-12.

These figures are presented only to illustrate the general variation in results among dust leachate evaporations. The spreadsheet provides the actual values.

Each leachate water composition is placed into the appropriate bin based on the above criteria. This process is repeated for all of the normalized leachate waters. The result is a set of six leachate composition bins; each populated with waters that yield chemically similar solutions after they are concentrated by evaporation.

The effectiveness of the binning process is evaluated in the same manner as the effectiveness of the seepage water binning process, as discussed in Section 6.6.4, by examining how well the process reduces the variability of important chemical parameters. Table 6.10-5b demonstrates that the binning procedure is effective in segregating the dust leachate water chemistries, where the effectiveness of the binning process can be evaluated by looking at the standard deviations in each group relative to the whole. For example, the overall standard deviation in pH of all the 25°C (77°F) and 65 percent relative humidity waters is 0.84, while the average of the standard deviations of those waters in the five bins is 0.06 (a factor of 14, Table 6.10-5b). The results for nitrate (reduced deviation by factor of 3), and to a lesser degree calcium and chloride (both with about a factor of 2 reduction in deviation), demonstrate that the binning process is effective.

Source: Output DTN: MO0310SPADL8U4.001.

Figure 6.10-7. Evaporated Water Compositions for Dust Leachate Bin 1 After Evaporation to 65 Percent Relative Humidity

Source: Output DTN: MO0310SPADLBU4.001.

Figure 6.10-8. Evaporated Water Compositions for Dust Leachate Bin 2 After Evaporation to 65 Percent Relative Humidity

Source: Output DTN: MO0310SPADLBU4.001.

Figure 6.10-9. Evaporated Water Compositions for Dust Leachate Bin 3 After Evaporation to 65 Percent Relative Humidity

Source: Output DTN: MO0310SPADLBU4.001.

Figure 6.10-10. Evaporated Water Compositions for Dust Leachate Bin 4 After Evaporation to 65 Percent Relative Humidity

Source: Output DTN: MO0310SPADLBU4.001.

Figure 6.10-11. Evaporated Water Compositions for Dust Leachate Bin 5 After Evaporation to 65 Percent Relative Humidity

Source: Output DTN: MO0310SPADLBU4.001.

Figure 6.10-12. Evaporated Water Compositions for Dust Leachate Bin 6 After Evaporation to 65 Percent Relative Humidity

Table 6.10-5a. Standard Deviation of Dust Leachate Water Chemistry After Evaporation to 65% RH, Before and After Binning

	Waters (n)	Standard Deviation of pH	Standard Deviation of Ca (mol/kg H ₂ O)	Standard Deviation of Cl (mol/kg H ₂ O)	Standard Deviation of NO ₃ (mol/kg H ₂ O)
Bin 1	3	0.10	0.64	0.47	0.77
Bin 2	4	0.01	<0.01	0.07	0.20
Bin 3	9	0.02	<0.01	0.24	0.36
Bin 4	12	0.14	0.01	0.25	1.66
Bin 5	23	0.05	<0.01	0.17	0.26
Bin 6	1	N/A	N/A	N/A	N/A
Average Bins 1 to 5 ^a		0.06	0.13	0.24	0.65
All Leachates, no binning		0.64	0.27	0.44	2.04

Source: Output DTN: MO0310SPADLBU4.001, EBS Dust Leachate Binning Abstraction Rev 01.xls.

NOTE: ^a These results are from hand calculations determining the average of the preceding bin values.

6.10.5.3 Choice of Representative Leachate Water for Each Bin

The “median” leachate water composition in each bin is chosen to represent all waters in that bin using the flagging methodology detailed in the next section. The “median” leachate water is a representative water as near the statistical median as possible. That is, this “median” water should be regarded as a representative “near-median” water composition and does not correspond to the actual statistical median for each individual chemical parameter. Table 6.10-6

gives the identifiers for the six median water compositions. Median equilibrated (calculated with the code EQ3NR) leachate water compositions for the bins are given in Table 6.10-9.

Table 6.10-6. Median Waters and Percentage of Waters in Each Bin

Bin	Median Water File Name	Number of Waters In the Bin	% of All Evaporated Waters Represented by the Bin
Bin 1	s80c25b.6o	3	5.77
Bin 2	s90b25b.6o	4	7.69
Bin 3	s86a25b.6o	9	17.31
Bin 4	p25_25b.6o	12	23.08
Bin 5	p26_25b.6o	23	44.23
Bin 6	s92a25b.6o	1	1.92
Total		52	100.00

Source: Output DTN: MO0310SPADLBU4.001, *EBS Dust Leachate Binning Abstraction Rev 01.xls*, Tab "Abstract Summary and Bin Stats."

All 52 waters found in the data and plots worksheet in *EBS Dust Leachate Binning Abstraction Rev 01.xls* (DTN: MO0310SPADLBU4.001) are sorted into six bins and copied into separate bin worksheets (e.g., Bin 1 abstract, Bin 2 abstract, etc.). These worksheets are used to determine the representative median water for each bin, as well as the individual bin statistics. In so doing, the 52 original waters are reduced to 6. These six water compositions are then used as inputs into Section 6.10.6 to create lookup tables for TSPA-LA analyses.

6.10.5.3.1 Median Water

The flagging methodology to determine the median water from each of the six bins uses the internal Excel functions of RANK and COUNTIF. These functions enable the selection of the median water by helping to determine and flag the actual middle value(s) for each parameter (e.g., pH, Ca, Cl) in each bin, and then counting the total number of these flagged values in each bin. Any ties are broken by flagging near-median values and summing the number of flags. This selection approach has the effect of maintaining consistency with the THC seepage abstraction outlined in Section 6.6. In addition, the selected bin chemistry is as close to the median chemistry within the bin as can be obtained without generating a hypothetical dust leachate water based on statistical averages of water constituent concentrations (Section 6.6.5.1). This approach minimizes potential errors because speciation calculations are often charge balanced by adjusting ions such as Na^+ or Cl^- , and adjusting the concentration of these ions could produce a brine that does not appropriately represent the bin waters. Table 6.10-6 lists the median waters selected for each bin.

6.10.5.3.2 Bin Distribution

The distribution of waters between the bins is calculated by determining the percentage of waters in each bin; this is shown on Table 6.10-6. Bin 5 contains the largest number of values and thus is the most probable water. Table 6.10-6 can be used to determine the relative probability of each dust leachate waters being present on drip shield and waste package surfaces in the absence of dripping (i.e., under deliquescence conditions). This is based on Assumption 5.2.1.

6.10.5.4 Within-Bin Uncertainty

In each of the six “bin abstract” worksheets, the median, minimum, and maximum values for each compositional parameter are calculated, as well as the standard deviation(s) and two standard deviations (2s). Table 6.10-7 contains the individual parameter statistics for each bin. These statistics are compared to those for all 52 dust leachate waters presented in Table 6.10-8. Comparison of Tables 6.10-7 and 6.10-8 indicate that the variation within each bin is generally much smaller than that observed for all 52 dust leachate waters.

6.10.5.5 EQ3NR Equilibrated Water Compositions

The six EQ3 input files associated with the calculated EQ6 output files listed in Table 6.10-6 have been used to represent the dust leachate compositions in the lookup table generation (Section 6.10.6.5). These six EQ3 3i files and the corresponding output files are archived in DTN: SN0310T0510102.010. Data from the six EQ3 3o files have been extracted using GETEQDATA Version 1.0.1 (BSC 2003 [DIRS 161900]) software to produce *6 bin EQ3 gas and dust leachate water extract.xls* (archived in DTN: MO0310SPADLBU4.001). This spreadsheet was then used to produce Tables 6.10-9 and 6.10-10, which represent the EQ3NR equilibration and charge balancing of the six chemistries listed on Table 6.10-6. The charge balance is done in accordance with the discussion in Section 6.10.3. EQ3NR is used only to equilibrate the solution with respect to all aqueous species. It does not equilibrate the solutions with respect to minerals and gases other than those discussed in Section 6.10.3. Subsequent EQ6 runs are used for additional mineral and gas phase equilibration.

6.10.5.6 Key Mineral Salt Assemblages

An abstraction of the dust samples into groups defined by their “key assemblages” is performed within *Environment on the Surfaces of the Drip Shield and Waste Package Outer Barrier* (BSC 2003 [DIRS 161237], Section 6.7.2.10). That report finds all dust samples can be represented by three key salt eutectic assemblages. Here the bin median dust samples are mapped to key assemblage representations in Table 6.10-10b.

Table 6.10-7. Calculated Statistics for Evaporated Dust Leachate Waters ($a_w = 0.65$) Within Each Bin

Bin	Statistic	pH	Br	C	Ca	Cl	F	K	Mg	N	Na	S	Si	Ionic Strength	Cl:N
1	Median	7.45	6.96E-02	5.04E-03	1.05E+00	3.28E+00	2.25E-05	1.17E+00	1.88E-01	6.79E+00	6.09E+00	5.48E-03	1.47E-05	11.27	0.55
	Min	7.31	2.73E-02	1.04E-03	3.37E-01	2.91E+00	2.16E-05	8.77E-01	5.62E-03	5.97E+00	4.59E+00	4.70E-03	1.25E-05	11.19	0.39
	Max	7.49	1.01E-01	6.74E-03	1.61E+00	3.84E+00	2.35E-05	1.70E+00	8.58E-01	7.51E+00	8.00E+00	1.09E-02	3.00E-04	12.11	0.56
	s	0.10	3.69E-02	2.93E-03	6.39E-01	4.66E-01	9.50E-07	4.16E-01	4.49E-01	7.67E-01	1.71E+00	3.38E-03	1.66E-04	0.51	0.10
	2s	0.19	7.39E-02	5.85E-03	1.28E+00	9.31E-01	1.90E-06	8.33E-01	8.97E-01	1.53E+00	3.42E+00	6.75E-03	3.31E-04	1.02	0.20
2	Median	7.94	2.68E+00	9.91E-04	9.61E-03	3.84E+00	1.39E-04	2.49E+00	7.74E-03	2.82E+00	7.28E+00	2.32E-01	4.89E-05	10.05	1.36
	Min	7.94	2.55E+00	7.58E-04	9.52E-03	3.71E+00	1.13E-04	2.35E+00	4.54E-03	2.78E+00	7.26E+00	2.31E-01	3.74E-05	10.04	1.16
	Max	7.96	2.70E+00	1.22E-03	9.67E-03	3.86E+00	1.66E-04	2.52E+00	1.05E-02	3.20E+00	7.56E+00	2.39E-01	6.18E-05	10.18	1.39
	s	0.01	6.96E-02	2.69E-04	7.92E-05	6.76E-02	3.05E-05	7.52E-02	3.35E-03	1.97E-01	1.45E-01	3.80E-03	1.37E-05	0.07	0.11
	2s	0.02	1.39E-01	5.39E-04	1.58E-04	1.35E-01	6.09E-05	1.50E-01	6.71E-03	3.94E-01	2.91E-01	7.60E-03	2.74E-05	0.14	0.21
3	Median	10.33	1.16E+00	4.49E-01	7.97E-06	4.18E+00	3.73E-02	3.55E+00	1.60E-05	2.85E+00	7.99E+00	1.24E+00	8.63E-04	13.16	1.47
	Min	10.32	1.14E+00	4.47E-01	7.97E-06	3.64E+00	2.58E-02	2.94E+00	2.56E-07	2.84E+00	7.97E+00	1.19E+00	5.11E-04	13.13	0.99
	Max	10.36	1.17E+00	4.52E-01	7.97E-06	4.18E+00	3.73E-02	3.55E+00	3.39E-05	3.66E+00	8.77E+00	1.25E+00	1.36E-02	13.28	1.47
	s	0.02	1.18E-02	1.88E-03	1.36E-09	2.37E-01	6.00E-03	2.69E-01	1.68E-05	3.61E-01	3.46E-01	2.40E-02	6.88E-03	0.06	0.21
	2s	0.03	2.37E-02	3.75E-03	2.71E-09	4.75E-01	1.20E-02	5.38E-01	3.36E-05	7.22E-01	6.92E-01	4.79E-02	1.38E-02	0.12	0.42
4	Median	8.29	4.71E-01	1.11E-03	7.05E-03	2.95E+00	1.36E-04	2.40E+00	2.28E-03	8.10E+00	1.01E+01	4.90E-01	1.92E-05	12.99	0.36
	Min	8.06	1.01E-01	3.63E-04	3.72E-03	2.75E+00	1.22E-04	2.15E+00	4.38E-05	4.67E+00	8.40E+00	2.94E-01	1.68E-05	10.88	0.30
	Max	8.51	1.88E+00	1.19E-03	8.87E-03	3.43E+00	1.99E-04	2.60E+00	6.55E-03	9.16E+00	1.07E+01	7.82E-01	7.51E-04	14.09	0.73
	s	0.14	6.65E-01	2.49E-04	1.36E-03	2.46E-01	2.81E-05	1.66E-01	1.68E-03	1.66E+00	8.41E-01	1.38E-01	2.10E-04	1.13	0.15
	2s	0.27	1.33E+00	4.97E-04	2.73E-03	4.93E-01	5.62E-05	3.32E-01	3.35E-03	3.33E+00	1.68E+00	2.76E-01	4.20E-04	2.25	0.31
5	Median	8.62	1.73E+00	1.33E-03	1.14E-03	3.65E+00	6.81E-04	2.92E+00	4.09E-04	3.55E+00	8.24E+00	1.12E+00	6.52E-05	12.28	1.03
	Min	8.62	1.70E+00	1.21E-03	4.97E-04	3.65E+00	4.68E-04	2.85E+00	3.71E-06	2.74E+00	7.47E+00	1.11E+00	3.96E-05	12.16	1.03
	Max	8.78	1.82E+00	2.16E-03	1.14E-03	4.21E+00	1.04E-03	3.64E+00	8.66E-04	3.55E+00	8.25E+00	1.23E+00	1.10E-03	12.38	1.54
	s	0.05	2.61E-02	2.63E-04	2.04E-04	1.69E-01	1.62E-04	2.19E-01	3.67E-04	2.58E-01	2.41E-01	3.72E-02	4.86E-04	0.05	0.16
	2s	0.10	5.22E-02	5.27E-04	4.08E-04	3.38E-01	3.23E-04	4.39E-01	7.33E-04	5.16E-01	4.82E-01	7.45E-02	9.71E-04	0.09	0.31
6	Median	10.27	1.54E+00	4.49E-01	7.87E-06	4.68E+00	3.59E-02	3.70E+00	2.55E-07	2.19E+00	7.07E+00	7.43E-01	1.28E-02	11.89	2.14
	Min														
	Max														
	s														
	2s														

Statistics are not defined for this bin that contains a single water chemistry

Source: Output DTN: MO0310SPADLBU4.001, EBS Dust Leachate Binning Abstraction Rev 01.xls.

NOTE: All units except for pH are in moles/kg $\times$ H₂O.

Table 6.10-8. Calculated Statistics for all 52 Evaporated Dust Leachate Waters Evaluated in the Binning Analysis ($a_w = 0.65$)

Statistic	pH	Br	C	Ca	Cl	F	K	Mg	N	Na	S	Si	Ionic Strength	Cl:N
Median	8.62	1.70E+00	1.33E-03	1.14E-03	3.65E+00	4.86E-04	2.92E+00	6.84E-04	3.55E+00	8.24E+00	1.12E+00	6.35E-05	1.23E+01	1.03
Min	7.31	2.73E-02	3.63E-04	7.87E-06	2.75E+00	2.16E-05	8.77E-01	2.55E-07	2.19E+00	4.59E+00	4.70E-03	1.25E-05	1.00E+01	0.30
Max	10.36	2.70E+00	4.52E-01	1.61E+00	4.68E+00	3.73E-02	3.70E+00	8.58E-01	9.16E+00	1.07E+01	1.25E+00	1.36E-02	1.41E+01	2.14
s	0.84	6.93E-01	1.78E-01	2.67E-01	4.37E-01	1.31E-02	5.86E-01	1.21E-01	2.04E+00	1.09E+00	4.16E-01	3.94E-03	9.35E-01	0.42
2s	1.69	1.39E+00	3.56E-01	5.34E-01	8.75E-01	2.61E-02	1.17E+00	2.42E-01	4.08E+00	2.18E+00	8.31E-01	7.89E-03	1.87E+00	0.83

Source: Output DTN: MO0310SPADLB4.001, EBS Dust Leachate Binning Abstraction Rev 01.xls, Tab "Data and Plots."

NOTE: All units except for pH are in moles/kg $\times$ H₂O.

Table 6.10-9. Total EQ3NR Equilibrated Aqueous Elemental Compositions for the 6 Bins

Bin	1	2	3	4	5	6
EQ3NR Filename	s80c25b.3o	s90b25b.3o	s86a25b.3o	p25_25b.3o	p26_25b.3o	s92a25b.3o
Temp (°C)	25	25	25	25	25	25
pH	8.54	8.09	8.23	8.54	8.40	8.05
a_w	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00
(I)	5.43E-03	2.74E-03	2.01E-03	6.29E-03	3.80E-03	1.15E-03
Br	5.01E-06	1.00E-05	3.75E-06	1.63E-05	1.63E-05	3.75E-06
C	1.96E-03	6.50E-04	8.86E-04	1.94E-03	1.36E-03	5.81E-04
Ca	1.35E-03	5.41E-04	3.09E-04	1.22E-03	7.17E-04	1.52E-04
Cl	2.17E-04	1.44E-04	1.35E-04	4.23E-04	2.82E-04	1.38E-04
F	3.16E-05	1.58E-05	1.58E-05	2.11E-05	3.68E-05	2.11E-05
K	2.63E-04	1.93E-04	2.99E-04	3.32E-04	2.63E-04	1.98E-04
Mg	1.65E-04	5.35E-05	4.81E-05	1.63E-04	7.08E-05	2.14E-05
N	5.16E-04	1.77E-04	1.18E-04	5.48E-04	3.23E-04	5.64E-05
Na	4.24E-04	4.05E-04	4.83E-04	1.34E-03	9.03E-04	3.72E-04
S	4.37E-04	3.96E-04	1.67E-04	6.97E-04	3.44E-04	6.04E-05
Si	1.46E-04	3.25E-05	6.27E-05	4.89E-05	7.91E-05	4.78E-05

Source: Output DTN: MO0310SPADLBU4.001, 6 bin EQ3 gas and dust leachate water extract.xls, Tab "Total Aqueous Elemental."

NOTE: Except for pH and a_w , all Units are in moles/kg $\times$ H₂O.

Table 6.10-10. EQ3NR Equilibrium Speciation of the Six Bins

Bin	1	2	3	4	5	6
Filename	s80c25b.3o	s90b25b.3o	s86a25b.3o	p25_25b.3o	p26_25b.3o	s92a25b.3o
HCO ₃ ⁻	1.84E-03	6.29E-04	8.61E-04	1.82E-03	1.31E-03	5.65E-04
Na ⁺	4.24E-04	4.05E-04	4.83E-04	1.34E-03	9.03E-04	3.72E-04
Ca ²⁺	1.26E-03	5.30E-04	3.02E-04	1.13E-03	6.87E-04	1.50E-04
SO ₄ ²⁻	4.25E-04	3.90E-04	1.65E-04	6.80E-04	3.38E-04	6.01E-05
NO ₃ ⁻	5.16E-04	1.77E-04	1.18E-04	5.48E-04	3.23E-04	5.64E-05
Cl ⁻	2.17E-04	1.44E-04	1.35E-04	4.23E-04	2.82E-04	1.38E-04
K ⁺	2.63E-04	1.93E-04	2.99E-04	3.33E-04	2.63E-04	1.98E-04
O _{2(aq)}	2.68E-04	2.68E-04	2.68E-04	2.68E-04	2.68E-04	2.68E-04
Mg ²⁺	1.60E-04	5.31E-05	4.75E-05	1.58E-04	6.93E-05	2.12E-05
CaCO _{3(aq)}	5.49E-05	3.04E-06	3.41E-06	4.69E-05	1.62E-05	7.84E-07
SiO _{2(aq)}	1.33E-04	3.14E-05	6.00E-05	4.46E-05	7.39E-05	4.64E-05
CO ₃ ²⁻	3.90E-05	4.32E-06	7.96E-06	3.87E-05	1.92E-05	3.34E-06
F ⁻	3.16E-05	1.58E-05	1.58E-05	2.11E-05	3.68E-05	2.11E-05
CaSO _{4(aq)}	1.26E-05	5.79E-06	1.49E-06	1.73E-05	6.02E-06	2.96E-07
CaHCO ₃ ⁺	1.91E-05	2.96E-06	2.38E-06	1.66E-05	7.71E-06	8.13E-07
Br ⁻	5.01E-06	1.00E-05	3.75E-06	1.63E-05	1.63E-05	3.75E-06
CO _{2(aq)}	1.07E-05	1.07E-05	1.07E-05	1.07E-05	1.07E-05	1.07E-05
HSiO ₃ ⁻	1.32E-05	1.06E-06	2.77E-06	4.38E-06	5.20E-06	1.40E-06
OH ⁻	3.85E-06	1.31E-06	1.80E-06	3.82E-06	2.74E-06	1.18E-06

Table 6.10-10. EQ3NR Equilibrium Speciation of the Six Bins (Continued)

Bin	1	2	3	4	5	6
MgCO _{3(aq)}	3.04E-06	1.34E-07	2.38E-07	2.84E-06	7.19E-07	4.94E-08
MgHCO ₃ ⁺	2.29E-06	2.83E-07	3.61E-07	2.18E-06	7.43E-07	1.11E-07
MgOH ⁺	9.03E-08	1.11E-08	1.42E-08	8.58E-08	2.93E-08	4.39E-09
CaOH ⁺	5.17E-08	8.03E-09	6.46E-09	4.50E-08	2.09E-08	2.21E-09
H ⁺	3.10E-09	8.68E-09	6.24E-09	3.16E-09	4.25E-09	9.28E-09
NaF _(aq)	1.14E-09	5.70E-10	6.92E-10	2.38E-09	2.91E-09	7.29E-10
HSO ₄ ⁻	8.95E-11	2.54E-10	7.97E-11	1.43E-10	1.03E-10	4.54E-11
NO ₂ ⁻	1.85E-17	6.33E-18	4.19E-18	1.96E-17	1.15E-17	2.01E-18
ClO ₄ ⁻	3.05E-27	2.02E-27	1.90E-27	5.94E-27	3.96E-27	1.94E-27
H _{2(aq)}	4.78E-45	4.78E-45	4.78E-45	4.78E-45	4.78E-45	4.78E-45
NH ₄ ⁺	8.13E-67	2.29E-66	7.97E-67	8.87E-67	9.77E-67	8.65E-67
NH _{3(aq)}	1.51E-67	1.51E-67	7.33E-68	1.61E-67	1.32E-67	5.35E-68

Source: Output DTN: MO0310SPADLBU4.001, 6 bin EQ3 gas and dust leachate water extract.xls, Tab "Aqueous Species."

NOTE: Units are in mol/kg × H₂O.

Table 6.10-10a. Median Bin Assignments and Correlation to Key Assemblages

Bin	Median Water File Name	Key Assemblage of Median Sample	Key Salts
Bin 1	s80c25b.6o	C	NaCl-KNO ₃ -NaNO ₃ -Ca(NO ₃) ₃ -KBr
Bin 2	s90b25b.6o	A	NaCl-KNO ₃ -KBr
Bin 3	s86a25b.6o	A	NaCl-KNO ₃ -KBr
Bin 4	p25 25b.6o	B	NaCl-KNO ₃ -NaNO ₃ -KBr
Bin 5	p26 25b.6o	A	NaCl-KNO ₃ -KBr
Bin 6	s92a25b.6o	A	NaCl-KNO ₃ -KBr

Sources: Table 6.10-6; BSC 2004 [DIRS 161237], Tables 6.7-9 and 6.7-11.

6.10.6 Development of Lookup Tables for Total System Performance Assessment - License Application

The lookup tables have been constructed based on the EQ3/6 (v. 8.0) calculations using thermodynamic database *data0.yprf* (Section 4.1.4, DTN: SN0302T0510102.002 [DIRS 162572]) and the USGS data on dust leachate compositions (DTNs: MO0207EBSDUSTS.020 [DIRS 162556], Table 4.1-19; MO0209EBSDUST2.030 [DIRS 162557], Table 4.1-20).

The model validation range for the current IDPS model is for temperatures up to 140°C (BSC 2004 [DIRS 169863]). The data are split into the calculation runs at 100°C and below (DTN: SN0310T0510102.011), and the calculation runs and lookup tables above this temperature (120°C and 140°C; DTN: SN0310T0510102.012).

6.10.6.1 Dust Leachate Water Inputs

Table 6.10-6 identifies the bin “median” composition inputs for the IDPS model calculations of aqueous solution compositions produced by deliquescence.

The EQ3NR input and output files for lookup table calculations are documented in DTN: SN0310T0510102.010. They are summarized in Table 6.10-11.

Table 6.10-11. EQ3NR Input/Output Files for TSPA-LA Dust Leachate Abstraction

Bin	Input File Names	Output File Names	Pickup File Names
1	<i>s80c25b.3i</i>	<i>s80c25b.3o</i>	<i>s80c25b.3p</i>
2	<i>s90b25b.3i</i>	<i>s90b25b.3o</i>	<i>s90b25b.3p</i>
3	<i>s86a25b.3i</i>	<i>s86a25b.3o</i>	<i>s86a25b.3p</i>
4	<i>p25_25b.3i</i>	<i>p25_25b.3o</i>	<i>p25_25b.3p</i>
5	<i>p26_25b.3i</i>	<i>p26_25b.3o</i>	<i>p26_25b.3p</i>
6	<i>s92a25b.3i</i>	<i>s92a25b.3o</i>	<i>s92a25b.3p</i>

Source: Output DTN: SN0310T0510102.010, directory EQ3_runs.

6.10.6.2 Temperature and Carbon Dioxide

Temperature and carbon dioxide fugacity are varied to capture the effects of these parameters on the evaporative evolution. Unlike the seepage lookup tables, deliquescence can occur at temperatures greater than 100°C in the repository. For temperature, the values are 40°C, 70°C, 100°C, 120°C, and 140°C. The CO₂ fugacity values are 10⁻², 10⁻³, and 10⁻⁴ bar. Each temperature is run for each CO₂ fugacity, resulting in fifteen combinations for each bin leachate. The input values for temperature and CO₂ fugacity are defined in the EQ6 input files of the IDPS model. These input files are based on the EQ6 input file templates of DTN: MO0303SPAMEQ36.000 [DIRS 162549]. The EQ3NR pickup files identified in Table 6.10-11 provided the bottom halves of the input files.

The IDPS model is used to generate lookup tables of water compositions produced by dust deliquescence over the expected range of in-drift relative humidity values for use in TSPA-LA calculations. To cover this range, the bin waters are typically evaporated to dryness (see Section 6.10.4 for the operational definition of dryness). The two exceptions are for the low temperature cases that were calculated down to 50 percent and 30 percent *RH* at 40°C and 70°C, respectively. These lower *RH* range limits were determined from the many waste package temperature/relative humidity plots in *Multiscale Thermohydrologic Model* (BSC 2004 [DIRS 169565], Section 6.3.1).

The starting bin waters are sufficiently dilute that they represented solutions in equilibrium with relative humidity between 99.9 and 99.99 percent. For potential relative humidity values higher than the starting bin water, condensation of water vapor is not simulated. The top value on any given lookup table should be sufficient to simulate the chemistry of the dilute waters above 99.99 percent. Thus, for each temperature and CO₂ fugacity combination, only one EQ6 input file is generated.

The resulting EQ6 input and output files for the bin waters are listed in Table 6.10-12 and documented in DTNs: SN0310T0510102.011 and SN0310T0510102.012. The file nomenclature is $d?c\#t\%.6i$ or $6o$, where “?” is the bin number (1, 2, etc.); “#” is 2, 3, or 4 for the partial pressure of CO_2 equal to 10^{-2} , 10^{-3} , or 10^{-4} bar, respectively; “%” is 04, 07, 10, 12, and 14, for temperature equal to 40°C , 70°C , 100°C , 120°C , and 140°C , respectively. For example, file $d1c2t10.6i$ is the dust EQ6 input file for bin 1 at 100°C and a fugacity of CO_2 of 10^{-2} bar.

Table 6.10-12. EQ6 Input/Output Files for TSPA-LA Abstraction

Bin	Input File Names	Output File Names
1	$d1c2t04.6i$, $d1c3t04.6i$, $d1c4t04.6i$, $d1c2t07.6i$, $d1c3t07.6i$, $d1c4t07.6i$, $d1c2t10.6i$, $d1c3t10.6i$, $d1c4t10.6i$, $d1c2t12.6i$, $d1c3t12.6i$, $d1c4t12.6i$, $d1c2t14.6i$, $d1c3t14.6i$, $d1c4t14.6i$	$d1c2t04.6o$, $d1c3t04.6o$, $d1c4t04.6o$, $d1c2t07.6o$, $d1c3t07.6o$, $d1c4t07.6o$, $d1c2t10.6o$, $d1c3t10.6o$, $d1c4t10.6o$, $d1c2t12.6o$, $d1c3t12.6o$, $d1c4t12.6o$, $d1c2t14.6o$, $d1c3t14.6o$, $d1c4t14.6o$
2	$d2c2t04.6i$, $d2c3t04.6i$, $d2c4t04.6i$, $d2c2t07.6i$, $d2c3t07.6i$, $d2c4t07.6i$, $d2c2t10.6i$, $d2c3t10.6i$, $d2c4t10.6i$, $d2c2t12.6i$, $d2c3t12.6i$, $d2c4t12.6i$, $d2c2t14.6i$, $d2c3t14.6i$, $d2c4t14.6i$	$d2c2t04.6o$, $d2c3t04.6o$, $d2c4t04.6o$, $d2c2t07.6o$, $d2c3t07.6o$, $d2c4t07.6o$, $d2c2t10.6o$, $d2c3t10.6o$, $d2c4t10.6o$, $d2c2t12.6o$, $d2c3t12.6o$, $d2c4t12.6o$, $d2c2t14.6o$, $d2c3t14.6o$, $d2c4t14.6o$
3	$d3c2t04.6i$, $d3c2t04b.6i$, $d3c3t04.6i$, $d3c4t04.6i$, $d3c2t07.6i$, $d3c3t07.6i$, $d3c4t07.6i$, $d3c2t10.6i$, $d3c2t10b.6i$, $d3c3t10.6i$, $d3c3t10b.6i$, $d3c4t10.6i$, $d3c4t10b.6i$, $d3c2t12.6i$, $d3c3t12.6i$, $d3c4t12.6i$, $d3c2t14.6i$, $d3c3t14.6i$, $d3c4t14.6i$	$d3c2t04.6o$, $d3c2t04b.6o$, $d3c3t04.6o$, $d3c4t04.6o$, $d3c2t07.6o$, $d3c3t07.6o$, $d3c4t07.6o$, $d3c2t10.6o$, $d3c2t10b.6o$, $d3c3t10.6o$, $d3c3t10b.6o$, $d3c4t10.6o$, $d3c4t10b.6o$, $d3c2t12.6o$, $d3c3t12.6o$, $d3c4t12.6o$, $d3c2t14.6o$, $d3c3t14.6o$, $d3c4t14.6o$
4	$d4c2t04.6i$, $d4c3t04.6i$, $d4c4t04.6i$, $d4c2t07.6i$, $d4c3t07.6i$, $d4c4t07.6i$, $d4c2t10.6i$, $d4c3t10.6i$, $d4c4t10.6i$, $d4c2t12.6i$, $d4c3t12.6i$, $d4c4t12.6i$, $d4c2t14.6i$, $d4c3t14.6i$, $d4c4t14.6i$	$d4c2t04.6o$, $d4c3t04.6o$, $d4c4t04.6o$, $d4c2t07.6o$, $d4c3t07.6o$, $d4c4t07.6o$, $d4c2t10.6o$, $d4c3t10.6o$, $d4c4t10.6o$, $d4c2t12.6o$, $d4c3t12.6o$, $d4c4t12.6o$, $d4c2t14.6o$, $d4c3t14.6o$, $d4c4t14.6o$
5	$d5c2t04.6i$, $d5c3t04.6i$, $d5c4t04.6i$, $d5c2t07.6i$, $d5c3t07.6i$, $d5c4t07.6i$, $d5c2t10.6i$, $d5c3t10.6i$, $d5c4t10.6i$, $d5c2t12.6i$, $d5c3t12.6i$, $d5c4t12.6i$, $d5c2t14.6i$, $d5c3t14.6i$, $d5c4t14.6i$	$d5c2t04.6o$, $d5c3t04.6o$, $d5c4t04.6o$, $d5c2t07.6o$, $d5c3t07.6o$, $d5c4t07.6o$, $d5c2t10.6o$, $d5c3t10.6o$, $d5c4t10.6o$, $d5c2t12.6o$, $d5c3t12.6o$, $d5c4t12.6o$, $d5c2t14.6o$, $d5c3t14.6o$, $d5c4t14.6o$
6	$d6c2t04.6i$, $d6c3t04.6i$, $d6c4t04.6i$, $d6c2t07.6i$, $d6c2t07b.6i$, $d6c3t07.6i$, $d6c4t07.6i$, $d6c2t10.6i$, $d6c2t10b.6i$, $d6c3t10.6i$, $d6c3t10b.6i$, $d6c4t10.6i$, $d6c4t10b.6i$, $d6c2t12.6i$, $d6c2t12b.6i$, $d6c3t12.6i$, $d6c3t12b.6i$, $d6c4t12.6i$, $d6c4t12b.6i$, $d6c2t14.6i$, $d6c2t14b.6i$, $d6c3t14.6i$, $d6c3t14b.6i$, $d6c4t14.6i$, $d6c4t14b.6i$	$d6c2t04.6o$, $d6c3t04.6o$, $d6c4t04.6o$, $d6c2t07.6o$, $d6c2t07b.6o$, $d6c3t07.6o$, $d6c4t07.6o$, $d6c2t10.6o$, $d6c2t10b.6o$, $d6c3t10.6o$, $d6c3t10b.6o$, $d6c4t10.6o$, $d6c4t10b.6o$, $d6c2t12.6o$, $d6c2t12b.6o$, $d6c3t12.6o$, $d6c3t12b.6o$, $d6c4t12.6o$, $d6c4t12b.6o$, $d6c2t14.6o$, $d6c2t14b.6o$, $d6c3t14.6o$, $d6c3t14b.6o$, $d6c4t14.6o$, $d6c4t14b.6o$

Source: Output DTNs: SN0310T0510102.011 and SN0310T0510102.012.

6.10.6.3 Calculation Using Additional Mineral and Aqueous SpeciesSuppressions

Additional mineral and aqueous species suppressions were used in some evaporation simulations of dust leachate waters at various temperatures. It was noted that the $\text{O}_{2(\text{aq})}$ concentration was reaching unreasonably high values at high levels of solute concentrations. This causes the EQ3/6 code calculation runs to terminate abruptly. This result seems to be a limitation of the *data0.yppf*

Pitzer database regarding this neutral species where its model parameters are bounded to lower ionic strengths. Conceptually, there is no reason for $O_{2(aq)}$ to concentrate to such levels under in-drift conditions, and the calculation code runs use a constant f_{O_2} value at 0.212 bars. Therefore, in cases where $O_{2(aq)}$ poses a problem, this species is suppressed, allowing the code calculation runs to proceed normally without affecting the values used to constrain f_{O_2} ; the gas phase O_2 controls redox reactions and not the aqueous phase. Table 6.10-13 shows the dust leachate water bins where this suppression was applied.

Table 6.10-13. AdditionalSuppressions and Inclusions in EQ3/6 Runs Involving Dust Leachate Evaporation as a Function of Temperature

Bin	Temperature (°C)	AdditionalSuppressions	Comments
Bins 1 to 6	40	None	—
Bins 1 to 4	70	None	—
Bin 5	70	$O_{2(aq)}$	—
Bin 6	70	$O_{2(aq)}$, natrite, and trona ^a	—
Bins 1, 2, 4, and 5	100	$O_{2(aq)}$	—
Bins 3 and 6	100	$O_{2(aq)}$, natrite, and trona ^a	Suppressions applied only to the extrapolation runs ^b
Bins 1, 2, 4, and 5	120	$O_{2(aq)}$	—
Bins 3 and 6	120	$O_{2(aq)}$, thermonatrite, and trona ^a	Suppressions applied only to the extrapolation runs ^b
Bins 1, 2, 4, and 5	140	$O_{2(aq)}$	—
Bins 3 and 6	140	$O_{2(aq)}$, thermonatrite	—

^a High temperature solubility data for Trona is absent from the database (only 25°C log K and extrapolation to >45°C are deemed unreliable.)

^b Extrapolation runs refer to those modified to attain the apparent eutectic nitrate salt assemblage (Section 6.10.6.4). These represented by files labeled ###b.3i and ###b.6i in output DTNs: SN0310T0510102.011 and SN0310T0510102.012.

Another suppression includes the mineral phases natrite and thermonatrite. These suppressions were applied to the code calculation runs only when these appear as saturated phases in the reaction path calculation. Natrite is suppressed in cases where it appears as part of the equilibrium mineral assemblage in reaction path calculations at temperatures below 100°C where thermonatrite is allowed to precipitate. Conversely, thermonatrite is suppressed in code calculation runs at 120°C and 140°C. The general rationale for this suppression is based on the occurrence and reported experimentally determined stability (Grønvold and Meisingset 1983 [DIRS 162069]) of these minerals at temperatures from 270 K to 400 K. Table 6.10-13 indicates the dust leachate water bins where these inclusions/suppressions for these Na-carbonate phases were implemented. The DTNs containing the associated EQ3/6 input/output files for these runs encompassing a temperature range of 40°C to 140°C are DTNs: SN0310T0510102.011 and SN0310T0510102.012.

6.10.6.4 EQ6 convergence Failures and Eutectic Point Estimation

Some evaporation simulations of the dust leachates fail to attain a eutectic point for the system K-Na-Cl- NO_3 . Eutectic salt assemblages in this system represent the nearest point to dryout in the evaporation run calculations. Prior to reaching this eutectic, a sulfate-chloride or

sulfate-carbonate salt assemblage is observed in Bins 3 and 6, at which point the EQ3/6 calculation fails to proceed further. To obtain the eutectic salt assemblage comprising components in the system K-Na-Cl-NO₃ for the dust leachate evaporation run calculations in these bins, an extrapolation was done from the convergence failure by taking the end-point chemistry for these cases and continuing the evaporation calculation from that point, but without the SO₄²⁻ species.

The removal of this component, whose concentration is non-negligible at the sulfate salt saturation point, requires the removal of Na⁺ and K⁺ to avoid charge imbalances. As Na⁺ and K⁺ are the dominant cations, and the saturation points of Na₂SO₄ and K₂SO₄ are similar, sodium and potassium were decreased in amounts equivalent to the molality of SO₄²⁻. Additional minor species were also dropped from the system at this point and charge balanced on K⁺. The end-point water compositions are used in a subsequent EQ3NR calculation run to generate a pickup file in order to continue the EQ6 solution evaporation.

In order to closely match the remaining mass of aqueous phase relative to the prior run (e.g., Appendix C, Figure C-03-05), the value for the aqueous phase scale factor in the new EQ3 #b.3i file was approximated to the mass of H₂O (in kg) remaining in the last step of the previous EQ6 calculation run. The effect of this is to scale down the initial amount of H₂O in the subsequent EQ6 calculation run, which is by default 1 kg. When these continuation-run calculations are combined for analysis with the initial evaporation results, the evaporation path is continued from the end-point activity water of the previous calculation run. This approach to extend from one salt equilibrium assemblage to another may be considered as a rough approximation. Nevertheless, the compositional differences are small when these are combined while closely matching the activity of H₂O in the preceding calculation. The solution compositions obtained by this method are within the compositional range of the observed values in the other evaporated water bins at the same temperature.

6.10.6.5 Lookup Tables

The results of the dust deliquescence abstractions that are to be used as direct input into TSPA-LA calculations are summarized in a set of lookup tables documented in DTNs: MO0310SPADLALT.001 and MO0310SPADLHTL.000. These lookup tables, listed in Table 6.10-14, include boundary conditions, abstraction output, and results of supplemental calculations. Each lookup table corresponds to one of the IDPS model output files identified in Table 6.10-12. Each row in these tables provides output parameter values as the water incrementally evolves due to evaporation or deliquescence given the defined boundary conditions. Each output row is defined by a unique equilibrium relative humidity.

The general lookup table format and the calculations in the lookup tables are developed and described in *In-Drift Precipitates/Salts Model* (BSC 2004 [DIRS 169863], Sections 6.7.3 and 6.6.3.5). The first three columns are reserved for the THC seepage lookup tables discussed in Section 6.9 and are not relevant for the dust leachate table analysis. The next column is the equilibrium relative humidity, calculated by multiplying the activity of water (listed in column K) by 100 percent. The rest of the columns are filled using GETEQDATA Version 1.0.1 (BSC 2003 [DIRS 161900]). Columns E through H show reaction progress and the boundary conditions for the starting water (i.e., the temperature and the fugacities of oxygen and carbon

dioxide). Columns I through X show reaction progress, pH, ionic strength, mass of H₂O in the reactor, and the total concentrations of the aqueous components. Columns Y through AL present reaction progress, mass of H₂O in the reactor, and the concentrations of potential acid-neutralizing species. Finally, columns AM through BD are reserved to show the amounts of minerals accumulated in the reactor. The values in the lookup tables may be used to define response surfaces so that interpolations or extrapolations may be obtained for precise input values not provided in the tables. Column E calculates the H₂O vapor pressure as a function of *RH* and the EQ6 calculated pressure (entered in Cell E1).

Table 6.10-14. Dust Leachate Evaporation Lookup Tables for TSPA-LA Abstraction

Bin	Lookup Tables
1	d1c2t04.xls, d1c3t04.xls, d1c4t04.xls d1c2t07.xls, d1c3t07.xls, d1c4t07.xls d1c2t10.xls, d1c3t10.xls, d1c4t10.xls d1c2t12.xls, d1c3t12.xls, d1c4t12.xls d1c2t14.xls, d1c3t14.xls, d1c4t14.xls
2	d2c2t04.xls, d2c3t04.xls, d2c4t04.xls d2c2t07.xls, d2c3t07.xls, d2c4t07.xls d2c2t10.xls, d2c3t10.xls, d2c4t10.xls d2c2t12.xls, d2c3t12.xls, d2c4t12.xls d2c2t14.xls, d2c3t14.xls, d2c4t14.xls
3	d3c2t04.xls, d3c3t04.xls, d3c4t04.xls d3c2t07.xls, d3c3t07.xls, d3c4t07.xls d3c2t10.xls, d3c3t10.xls, d3c4t10.xls d3c2t12.xls, d3c3t12.xls, d3c4t12.xls d3c2t14.xls, d3c3t14.xls, d3c4t14.xls
4	d4c2t04.xls, d4c3t04.xls, d4c4t04.xls d4c2t07.xls, d4c3t07.xls, d4c4t07.xls d4c2t10.xls, d4c3t10.xls, d4c4t10.xls d4c2t12.xls, d4c3t12.xls, d4c4t12.xls d4c2t14.xls, d4c3t14.xls, d4c4t14.xls
5	d5c2t04.xls, d5c3t04.xls, d5c4t04.xls d5c2t07.xls, d5c3t07.xls, d5c4t07.xls d5c2t10.xls, d5c3t10.xls, d5c4t10.xls d5c2t12.xls, d5c3t12.xls, d5c4t12.xls d5c2t14.xls, d5c3t14.xls, d5c4t14.xls
6	d6c2t04.xls, d6c3t04.xls, d6c4t04.xls d6c2t07.xls, d6c3t07.xls, d6c4t07.xls d6c2t10.xls, d6c3t10.xls, d6c4t10.xls d6c2t12.xls, d6c3t12.xls, d6c4t12.xls d6c2t14.xls, d6c3t14.xls, d6c4t14.xls

Source: Output DTNs: MO0310SPADLALT.001 and MO0310SPADLHTL.000.

6.10.7 Illustration of Results

Figures 6.10-13 through 6.10-18 graphically illustrate the results with plotted values from the *d5c3t7.xls* lookup table. These figures are meant to illustrate the general output trends; for actual values, consult the lookup tables directly. These are bin 5 evaporation results at a temperature of 70°C and a CO₂ fugacity of 10⁻³ bar. The first two plot the total elemental aqueous concentrations and pH as a function of relative humidity and concentration factor. The next two plot the ANC aqueous species concentrations (HCO₃⁻, CO₃²⁻, HSiO₃⁻, CaHCO₃⁺, OH⁻,

MgHCO_3^+ , H^+ , MgOH^+ , CaOH^+ , HSO_4^- , Ca^{2+} , and Mg^{2+}) and pH as functions of relative humidity and concentration factor. The last two results plot pH, the fixed CO_2 and O_2 fugacity, and the moles of minerals precipitated from one kilogram of dust condensate water as a function of relative humidity and concentration factor. The graphical results from the remainder of the lookup tables are provided in Appendix C.

6.10.8 Correction of SiO_2 Concentration Units: Sensitivity Analysis of Dust Leachate Evaporation

Concentration of Si content in the dust leachate waters is expressed in ppm (e.g., mg of solute per kg of solvent H_2O). However, Si concentration is entered as $\text{SiO}_{2(\text{aq})}$ in the EQ3/6 input files. Therefore, a conversion from Si to SiO_2 in ppm units is needed to correctly represent the concentration of this component in the code run calculations. This step was inadvertently omitted during the calculation of input leachate concentrations for the EQ3/6 calculation runs given in DTN: SN0310T0510102.010 (Sections 6.10.3 and 6.10.4). Because of this, a sensitivity analysis based on a comparison between a corrected and an uncorrected Si concentration unit has been done using the six dust leachate median bin water values listed on Table 6.10.6. A comparison of resulting outputs is given in DTN: MO0311SPASADLS.000.

Source: Output DTN: MO0310SPADLALT.001.

Figure 6.10-13. Predicted Evolution of Dust Leachate Bin 5 Water Evaporated at 70°C and 10^{-3} Bar CO_2 Fugacity.

Source: Output DTN: MO0310SPADLALT.001.

Figure 6.10-14. Predicted Evolution of Dust Leachate Bin 5 Water Evaporated at 70°C and 10^{-3} Bar CO_2 Fugacity.

Source: Output DTN: MO0310SPADLALT.001.

Figure 6.10-15. Predicted Concentrations of ANC Species During Evaporation of Dust Leachate Bin 5 Water at 70°C and 10^{-3} Bar CO_2 Fugacity.

Source: Output DTN: MO0310SPADLALT.001.

Figure 6.10-16. Predicted Concentrations of ANC Species During Evaporation of Dust Leachate Bin 5 Water at 70°C and 10^{-3} Bar CO_2 Fugacity.

Source: Output DTN: MO0310SPADLALT.001.

Figure 6.10-17. Predicted Mineral Precipitation during evaporation of Dust Leachate Bin 5 Water at 70°C and 10^{-3} Bar CO_2 Fugacity.

Source: Output DTN: MO0310SPADLALT.001.

Figure 6.10-18. Predicted Mineral Precipitation during evaporation of Dust Leachate Bin 5 Water at 70°C and 10-3 Bar CO₂ Fugacity.

A priori, it is not expected that this change in Si concentration during evaporation down to an activity of water of ~ 0.65 would affect the output results in a significant way, because of its relatively low concentration in the starting water compositions. Mg^{2+} concentrations are slightly different in most calculation runs due to sepiolite formation, except in the median waters p25 and S92a, where the resulting concentrations are similar. In water S80c, the predicted values for pH and the concentrations of Ca^{2+} and SO_4^{2-} differ in the calculation runs using the corrected and uncorrected $\text{SiO}_{2(aq)}$ concentrations. In both cases, similar Si phases with relatively low solubilities form early in the evaporation simulation and the common Si phase added to the equilibrium mineral assemblages in the early stages of the evaporation is sepiolite. However, due to the larger amount of Si in the calculation run with the corrected SiO_2 concentration (S80c_25bt), more sepiolite precipitates, resulting in the reduction of Mg in solution. This decrease in Mg prevents saturation with respect to huntite, a Ca-Mg carbonate phase which precipitates in the uncorrected $\text{SiO}_{2(aq)}$ run. In the uncorrected case, saturation with respect to this phase causes a further decrease in Ca, that in turn affects the SO_4^{2-} equilibrium concentration with respect to gypsum – a common phase in both calculation runs. Moreover, saturation with respect to huntite also affects the HCO_3^- concentration (because it affects the amount of CaCO_3 that precipitates), causing the pH to be slightly higher (~ 0.2 pH units, well within the uncertainty range in bin 1 pH values, Table 6.12-8). In the S80c simulation using the corrected $\text{SiO}_{2(aq)}$ concentration, relatively larger amounts of sepiolite formed, reducing total Mg concentration and preventing the formation of huntite. The only median water affected by the change in the input values for $\text{SiO}_{2(aq)}$ is S80c, which is present in bin 1, and which only comprises ~ 5 percent of all the dust leachate waters. Therefore, the use of the incorrect Si content in the dust leachates will not significantly impact chemical parameters relevant to TSPA-LA models, such as Cl/NO₃ ratios.

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 169856]). 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

determined by chemical divides or mineralogy of precipitates. A cluster is defined as “a group of THC model precipitated minerals,” which is not chosen by physical/chemical criteria (as in “binning”) but is instead chosen using “cluster analysis” in the Statistica 5.1 software.

6.11.1.1 Clustering Based on Mineralogy

The analysis begins by taking the mineral data from each EQ3/6 output from *EBS THC Seepage Binning Abstraction REV 4.xls* developed in Section 6.6.4 and archived in DTN: MO0310SPAEBSCB.003. For abstraction purposes, only data from the carbonate, chloride, nitrate, and sulfate phases are used; the silicate and fluoride minerals are excluded from the clustering investigation. The mineral phases used for the clustering case are:

- anhydrite (CaSO_4)
- arcanite (K_2SO_4)
- calcite (CaCO_3)
- darapskite ($\text{Na}_3\text{NO}_3\text{SO}_4 \cdot \text{H}_2\text{O}$)
- glauberite ($\text{Na}_2\text{Ca}(\text{SO}_4)_2$)
- halite (NaCl)
- nahcolite (NaHCO_3)
- natrite (Na_2CO_3)
- niter (KNO_3)
- pentasalt ($\text{K}_2\text{SO}_4 \cdot 5\text{CaSO}_4 \cdot \text{H}_2\text{O}$)
- thenardite (Na_2SO_4)
- trona ($\text{Na}_3\text{HCO}_3\text{CO}_3 \cdot \text{H}_2\text{O}$).

Values for all of the selected minerals (moles precipitated) are cut and pasted from *EBS THC Seepage Binning Abstraction REV 4.xls* into a Statistica 5.1 main data file/spreadsheet (NewQminbin.STA, archived in DTN: MO0310SPAPCEAC.002). This is the main data file from which the cluster analysis is developed. This data is binned using a “K-means cluster analysis.” In cluster sampling, clusters of individual units are chosen at random, and all units in the chosen clusters are measured (Gilbert 1987 [DIRS 163705], p. 23). In a K-means cluster analysis, the user is allowed to select the number of clusters to form. Eleven clusters have been chosen for the model simply because 11 bins are used in the aqueous binning abstraction, thus a more direct comparison can be made between the uncertainty of the solute concentrations (including pH) in the waters of the 11 bins within the aqueous abstraction with the uncertainty of the solute concentration in the waters of each of the 11 clusters comprising the mineral abstraction. For the cluster analysis, output data is saved in Statistica 5.1 files (Table 6.11-1). All 368 waters (called case numbers by Statistica 5.1) from *EBS THC Seepage Binning Abstraction REV 4.xls* are assigned a cluster (1-11) by cluster analysis in Statistica 5.1. For each specified cluster, case numbers are determined by checking the Statistica 5.1 output files *WATERS OF CLUSTER NO 1.SCR* to *WATERS OF CLUSTER NO 11.SCR* (archived in DTN: MO0310SPAPCEAC.002). The statistics mean and standard deviation are then calculated for each solute concentration and pH to determine the uncertainty for each cluster (*New Mineral Binning Stats2.xls*). These uncertainties are then compared to the uncertainty of the 11-bin aqueous abstraction by determining the mean coefficient of variation for both the mineral clustering and aqueous binning for each solute and pH (Tables 6.11-3 to 6.11-14). The associated

precipitated minerals (excluding silicates and fluorides) for each of the 11 clusters are given in Table 6.11-2.

Table 6.11-1. Statistica 5.1 Files Saved from Generated Data

11-Cluster Model
<i>NewQminbin.STA</i>
<i>WATERS OF CLUSTER NO 1.SCR to WATERS OF CLUSTER NO 11.SCR</i>

Source: Output DTN: MO0310SPAPCEAC.002.

6.11.1.2 Results

Results shown in Tables 6.11-3 to 6.11-14 indicate that the coefficients of variation are lower for aqueous binning in 6 cases and lower for mineral clustering in 6 cases. The mean value of the coefficients of variation is smaller for the solute species Ca, F, N, S, Si, and pH in the 11-bin aqueous abstraction. The mean value of the coefficient of variations is smaller for Al, C, Cl, K, Mg, and Na for the 11-cluster mineral case. On the basis of these results, where pH, Ca, N, F, and S uncertainties (mean coefficient of variations) are lower for the aqueous binning case and the Cl uncertainty (mean coefficient of variation) is very similar, the mineral clustering approach has been discarded in favor of the aqueous composition binning approach. However, because the results are similar, the alternate method corroborates the chosen method.

Table 6.11-2. Clusters 1-11 with Associated Minerals

Mineral	Cluster 1	Cluster 2	Cluster 3	Cluster 4	Cluster 5	Cluster 6	Cluster 7	Cluster 8	Cluster 9	Cluster 10	Cluster 11
Anhydrite	-	-	-	-	-	-	-	X	-	-	-
Arcanite	X	X	-	-	-	X	X	-	X	X	X
Calcite	-	-	X	-	X	X	-	X	X	-	X
Darapskite	-	-	-	-	-	-	-	-	-	-	X
Glauberite	-	-	-	-	-	X	-	X	-	-	-
Halite	X	-	X	-	-	X	X	X	X	-	X
Nahcolite	-	X	-	-	-	X	X	-	X	-	X
Natrite	-	X	X	X	X	X	X	-	-	X	-
Niter	-	-	-	-	-	-	-	-	-	-	X
Pentasalt	-	-	-	-	-	-	-	X	-	-	-
Thenardite	X	X	X	-	X	X	X	-	X	X	X
Trona	X	-	-	-	-	-	-	-	-	X	-

Source: Output DTN: MO0310SPAPCEAC.002; New Mineral Binning Stats2.xls.

Table 6.11-3. pH Statistics for Mineral Clustering and Aqueous Binning

pH by Mineral Clustering					pH by Aqueous Binning				
Cluster	Waters (n)	Mean	Standard Deviation	% Coefficient of Variation	Bin	Waters (n)	Mean	Standard Deviation	% Coefficient of Variation
Cluster 1	4	9.09	0.02	0.26	Bin 1	5	5.62	0.08	1.35
Cluster 2	6	9.27	0.19	2.10	Bin 2	13	5.66	0.11	1.91
Cluster 3	80	9.15	0.17	1.88	Bin 3	12	5.89	0.24	4.14
Cluster 4	12	9.23	0.22	2.43	Bin 4	43	7.05	0.34	4.80
Cluster 5	32	9.24	0.18	1.97	Bin 5	27	7.64	0.29	3.82
Cluster 6	45	8.22	0.78	9.54	Bin 6	8	9.05	0.37	4.04
Cluster 7	24	8.86	0.10	1.15	Bin 7	25	8.74	0.16	1.81
Cluster 8	73	6.51	0.71	10.84	Bin 8	22	8.61	0.14	1.63
Cluster 9	36	8.70	0.19	2.15	Bin 9	58	9.13	0.22	2.36
Cluster 10	46	9.29	0.18	1.97	Bin 10	10	8.79	0.10	1.17
Cluster 11	10	8.67	0.15	1.77	Bin 11	145	9.21	0.19	2.05
Mean				3.28	Mean				2.64

Source: Output DTN: MO0310SPAPCEAC.002; New Mineral Binning Stats2.xls.

Table 6.11-4. AI Statistics for Mineral Clustering and Aqueous Binning

AI by Mineral Clustering (Moles/kg H ₂ O)					AI by Aqueous Binning (Moles/kg H ₂ O)				
Cluster	Waters (n)	Mean	Standard Deviation	% Coefficient of Variation	Bin	Waters (n)	Mean	Standard Deviation	% Coefficient of Variation
Cluster 1	4	2.13E-14	1.62E-15	7.57	Bin 1	5	3.26E-12	2.22E-13	6.81
Cluster 2	6	1.22E-13	6.49E-14	53.13	Bin 2	13	2.52E-12	7.15E-13	28.36
Cluster 3	80	1.25E-13	6.43E-14	51.52	Bin 3	12	1.15E-12	9.64E-13	83.90
Cluster 4	12	9.96E-12	3.34E-11	335.89	Bin 4	43	3.28E-13	2.78E-13	84.62
Cluster 5	32	1.31E-13	7.11E-14	54.46	Bin 5	27	1.66E-13	8.09E-14	48.63
Cluster 6	45	1.61E-13	1.04E-13	64.81	Bin 6	8	1.10E-13	9.15E-14	83.18
Cluster 7	24	1.51E-14	1.09E-14	71.83	Bin 7	25	4.11E-15	1.08E-15	26.19
Cluster 8	73	1.05E-12	1.15E-12	108.82	Bin 8	22	1.33E-15	6.66E-16	50.25
Cluster 9	36	4.05E-15	2.59E-15	64.06	Bin 9	58	2.18E-12	1.52E-11	698.63
Cluster 10	46	9.54E-14	3.23E-14	33.90	Bin 10	10	9.78E-15	3.33E-15	34.06
Cluster 11	10	6.92E-16	4.62E-18	0.67	Bin 11	145	1.00E-13	4.21E-14	41.88
Mean				76.97	Mean				107.87

Source: Output DTN: MO0310SPAPCEAC.002; New Mineral Binning Stats2.xls.

Table 6.11-5. C Statistics for Mineral Clustering and Aqueous Binning

C by Mineral Clustering (Moles/kg H ₂ O)					C by Aqueous Binning (Moles/kg H ₂ O)				
Cluster	Waters (n)	Mean	Standard Deviation	% Coefficient of Variation	Bin	Waters (n)	Mean	Standard Deviation	% Coefficient of Variation
Cluster 1	4	1.15E+00	9.50E-03	0.82	Bin 1	5	5.37E-04	8.67E-05	16.15
Cluster 2	6	1.32E+00	1.58E-01	11.95	Bin 2	13	6.04E-04	1.52E-04	25.12
Cluster 3	80	1.13E+00	4.41E-02	3.89	Bin 3	12	5.02E-04	1.84E-04	36.55
Cluster 4	12	1.29E+00	8.25E-02	6.40	Bin 4	43	5.04E-04	3.15E-04	62.43
Cluster 5	32	1.19E+00	1.71E-01	14.37	Bin 5	27	2.81E-03	5.84E-03	208.21
Cluster 6	45	2.62E-01	3.86E-01	147.17	Bin 6	8	5.07E-01	2.52E-01	49.71
Cluster 7	24	6.63E-01	2.85E-01	42.98	Bin 7	25	3.71E-01	1.06E-01	28.50
Cluster 8	73	5.24E-04	2.62E-04	50.02	Bin 8	22	2.08E-01	3.28E-02	15.82
Cluster 9	36	3.57E-01	1.68E-01	46.98	Bin 9	58	1.10E+00	2.12E-01	19.33
Cluster 10	46	1.25E+00	1.34E-01	10.72	Bin 10	10	4.03E-01	7.77E-02	19.26
Cluster 11	10	1.92E-01	3.64E-02	18.93	Bin 11	145	1.18E+00	1.35E-01	11.43
Mean				32.20	Mean				44.77

Source: Output DTN: MO0310SPAPCEAC.002; New Mineral Binning Stats2.xls.

Table 6.11-6. Ca Statistics for Mineral Clustering and Aqueous Binning

Ca by Mineral Clustering (Moles/kg H ₂ O)					Ca by Aqueous Binning (Moles/kg H ₂ O)				
Cluster	Waters (n)	Mean	Standard Deviation	% Coefficient of Variation	Bin	Waters (n)	Mean	Standard Deviation	% Coefficient of Variation
Cluster 1	4	2.69E-06	4.98E-08	1.85	Bin 1	5	3.66E+00	2.88E-01	7.87
Cluster 2	6	2.49E-06	1.23E-07	4.93	Bin 2	13	2.37E+00	2.75E-01	11.63
Cluster 3	80	4.25E-06	2.15E-06	50.58	Bin 3	12	1.12E+00	4.24E-01	37.87
Cluster 4	12	2.60E-06	1.28E-07	4.91	Bin 4	43	2.63E-03	6.45E-04	24.54
Cluster 5	32	3.00E-06	1.26E-06	42.04	Bin 5	27	8.20E-04	1.72E-04	20.97
Cluster 6	45	4.95E-04	4.24E-04	85.51	Bin 6	8	8.31E-06	5.58E-07	6.72
Cluster 7	24	1.21E-06	7.20E-07	59.66	Bin 7	25	9.88E-06	7.70E-07	7.80
Cluster 8	73	8.58E-01	1.20E+00	140.33	Bin 8	22	1.15E-05	1.38E-06	11.97
Cluster 9	36	1.03E-05	1.22E-06	11.81	Bin 9	58	3.33E-06	1.98E-06	59.49
Cluster 10	46	2.62E-06	1.07E-07	4.09	Bin 10	10	5.46E-07	1.55E-07	28.40
Cluster 11	10	1.16E-05	1.75E-06	15.10	Bin 11	145	3.51E-06	1.81E-06	51.66
Mean				38.25	Mean				24.45

Source: Output DTN: MO0310SPAPCEAC.002; New Mineral Binning Stats2.xls.

Table 6.11-7. CI Statistics for Mineral Clustering and Aqueous Binning

CI by Mineral Clustering (Moles/kg H ₂ O)					CI by Aqueous Binning (Moles/kg H ₂ O)				
Cluster	Waters (n)	Mean	Standard Deviation	% Coefficient of Variation	Bin	Waters (n)	Mean	Standard Deviation	% Coefficient of Variation
Cluster 1	4	6.22E+00	5.48E-01	8.81	Bin 1	5	8.14E+00	9.19E-01	11.29
Cluster 2	6	6.27E+00	4.92E-01	7.85	Bin 2	13	7.93E+00	6.77E-01	8.53
Cluster 3	80	6.29E+00	7.83E-01	12.46	Bin 3	12	8.30E+00	4.04E-01	4.87
Cluster 4	12	5.31E+00	2.23E-01	4.21	Bin 4	43	6.32E+00	1.87E+00	29.57
Cluster 5	32	6.03E+00	7.74E-01	12.82	Bin 5	27	7.63E+00	3.23E-01	4.24
Cluster 6	45	6.81E+00	1.46E+00	21.44	Bin 6	8	6.08E+00	1.65E+00	27.07
Cluster 7	24	5.84E+00	6.45E-01	11.04	Bin 7	25	5.68E+00	5.03E-01	8.85
Cluster 8	73	7.06E+00	1.73E+00	24.50	Bin 8	22	4.67E+00	7.31E-01	15.67
Cluster 9	36	5.70E+00	3.70E-01	6.50	Bin 9	58	5.27E+00	6.09E-01	11.56
Cluster 10	46	6.40E+00	4.48E-01	7.00	Bin 10	10	5.42E+00	4.98E-01	9.19
Cluster 11	10	4.21E+00	7.41E-01	17.62	Bin 11	145	6.56E+00	3.93E-01	5.99
Mean				12.20	Mean				12.44

Source: Output DTN: MO0310SPAPCEAC.002; New Mineral Binning Stats2.xls.

Table 6.11-8. F Statistics for Mineral Clustering and Aqueous Binning

F by Mineral Clustering (Moles/kg H ₂ O)					F by Aqueous Binning (Moles/kg H ₂ O)				
Cluster	Waters (n)	Mean	Standard Deviation	% Coefficient of Variation	Bin	Waters (n)	Mean	Standard Deviation	% Coefficient of Variation
Cluster 1	4	2.24E-01	5.25E-04	0.23	Bin 1	5	6.36E-05	4.18E-06	6.58
Cluster 2	6	2.52E-01	1.47E-02	5.83	Bin 2	13	5.07E-05	3.50E-06	6.89
Cluster 3	80	2.07E-01	4.51E-02	21.77	Bin 3	12	4.23E-05	1.36E-05	32.15
Cluster 4	12	2.44E-01	6.94E-03	2.84	Bin 4	43	7.66E-04	2.50E-04	32.64
Cluster 5	32	2.39E-01	3.27E-02	13.71	Bin 5	27	2.94E-03	3.24E-03	110.06
Cluster 6	45	3.98E-02	5.25E-02	131.75	Bin 6	8	7.83E-02	1.63E-02	20.81
Cluster 7	24	2.17E-01	9.52E-03	4.39	Bin 7	25	4.49E-02	1.15E-02	25.59
Cluster 8	73	4.71E-04	4.03E-04	85.49	Bin 8	22	2.26E-02	4.79E-03	21.18
Cluster 9	36	4.24E-02	1.91E-02	45.01	Bin 9	58	2.19E-01	4.11E-02	18.82
Cluster 10	46	2.51E-01	1.25E-02	4.99	Bin 10	10	2.09E-01	2.71E-03	1.30
Cluster 11	10	1.89E-02	3.42E-03	18.06	Bin 11	145	2.26E-01	4.22E-02	18.71
Mean				30.37	Mean				26.79

Source: Output DTN: MO0310SPAPCEAC.002; New Mineral Binning Stats2.xls.

Table 6.11-9. K Statistics for Mineral Clustering and Aqueous Binning

K by Mineral Clustering (Moles/kg H ₂ O)					K by Aqueous Binning (Moles/kg H ₂ O)				
Cluster	Waters (n)	Mean	Standard Deviation	% Coefficient of Variation	Bin	Waters (n)	Mean	Standard Deviation	% Coefficient of Variation
Cluster 1	4	4.01E+00	3.04E-02	0.76	Bin 71	5	3.11E-01	1.13E-01	36.29
Cluster 2	6	4.74E+00	7.92E-01	16.70	Bin 2	13	9.75E-01	3.32E-01	34.08
Cluster 3	80	3.62E+00	2.42E-01	6.69	Bin 3	12	3.07E+00	9.15E-01	29.78
Cluster 4	12	5.06E+00	5.35E-01	10.58	Bin 4	43	5.38E+00	9.45E-01	17.57
Cluster 5	32	3.94E+00	4.02E-01	10.19	Bin 5	27	4.69E+00	6.75E-02	1.44
Cluster 6	45	4.33E+00	5.96E-01	13.76	Bin 6	8	4.05E+00	6.66E-01	16.44
Cluster 7	24	4.39E+00	2.35E-01	5.35	Bin 7	25	4.85E+00	2.40E-01	4.96
Cluster 8	73	3.87E+00	2.13E+00	54.99	Bin 8	22	4.61E+00	6.63E-01	14.39
Cluster 9	36	4.94E+00	2.16E-01	4.37	Bin 9	58	4.03E+00	8.45E-01	20.99
Cluster 10	46	4.31E+00	2.15E-01	4.98	Bin 10	10	4.59E+00	4.66E-02	1.02
Cluster 11	10	4.05E+00	5.89E-01	14.53	Bin 11	145	3.98E+00	3.30E-01	8.30
Mean				12.99	Mean				16.84

Source: Output DTN: MO0310SPAPCEAC.002; New Mineral Binning Stats2.xls.

Table 6.11-10. Mg Statistics for Mineral Clustering and Aqueous Binning

Mg by Mineral Clustering (Moles/kg H ₂ O)					Mg by Aqueous Binning (Moles/kg H ₂ O)				
Cluster	Waters (n)	Mean	Standard Deviation	% Coefficient of Variation	Bin	Waters (n)	Mean	Standard Deviation	% Coefficient of Variation
Cluster 1	4	2.20E-07	1.89E-08	8.56	Bin 1	5	8.38E-04	3.55E-04	42.40
Cluster 2	6	6.95E-08	9.94E-08	143.07	Bin 2	13	1.39E-03	5.87E-04	42.27
Cluster 3	80	6.28E-08	6.17E-08	98.31	Bin 3	12	1.30E-03	7.39E-04	57.05
Cluster 4	12	6.70E-08	8.30E-08	123.87	Bin 4	43	2.16E-05	8.23E-05	381.32
Cluster 5	32	4.87E-08	6.35E-08	130.48	Bin 5	27	2.09E-06	2.37E-06	113.35
Cluster 6	45	1.36E-06	2.06E-06	151.46	Bin 6	8	1.66E-07	1.91E-07	115.42
Cluster 7	24	4.21E-07	8.96E-08	21.30	Bin 7	25	1.26E-06	5.78E-07	45.93
Cluster 8	73	5.30E-04	7.37E-04	139.01	Bin 8	22	2.72E-06	1.21E-06	44.52
Cluster 9	36	1.67E-06	1.05E-06	62.59	Bin 9	58	1.16E-07	1.65E-07	141.39
Cluster 10	46	5.50E-08	6.03E-08	109.72	Bin 10	10	4.30E-07	8.62E-08	20.03
Cluster 11	10	2.80E-06	1.45E-06	51.55	Bin 11	145	7.29E-08	8.18E-08	112.26
Mean				94.54	Mean				101.45

Source: Output DTN: MO0310SPAPCEAC.002; New Mineral Binning Stats2.xls.

Table 6.11-11. N Statistics for Mineral Clustering and Aqueous Binning

N by Mineral Clustering (Moles/kg H ₂ O)					N by Aqueous Binning (Moles/kg H ₂ O)				
Cluster	Waters (n)	Mean	Standard Deviation	% Coefficient of Variation	Bin	Waters (n)	Mean	Standard Deviation	% Coefficient of Variation
Cluster 1	4	1.01E+00	8.44E-01	83.35	Bin 1	5	8.88E-01	1.05E+00	118.66
Cluster 2	6	8.46E-01	6.79E-01	80.26	Bin 2	13	1.16E+00	8.35E-01	72.23
Cluster 3	80	1.22E+00	1.22E+00	99.31	Bin 3	12	1.25E+00	5.58E-01	44.56
Cluster 4	12	2.25E+00	9.52E-02	4.24	Bin 4	43	4.76E+00	2.79E+00	58.72
Cluster 5	32	1.32E+00	9.88E-01	74.85	Bin 5	27	1.28E+00	5.63E-01	43.89
Cluster 6	45	2.02E+00	1.92E+00	95.30	Bin 6	8	2.55E+00	2.73E+00	106.79
Cluster 7	24	2.25E+00	1.15E+00	51.00	Bin 7	25	3.00E+00	8.14E-01	27.17
Cluster 8	73	3.28E+00	2.83E+00	86.25	Bin 8	22	4.37E+00	1.43E+00	32.69
Cluster 9	36	2.93E+00	6.74E-01	23.00	Bin 9	58	2.70E+00	9.15E-01	33.89
Cluster 10	46	5.13E-01	7.58E-02	14.78	Bin 10	10	3.22E+00	8.54E-01	26.50
Cluster 11	10	4.78E+00	1.92E+00	40.21	Bin 11	145	5.71E-01	1.52E-01	26.63
Mean				59.32	Mean				53.79

Source: Output DTN: MO0310SPAPCEAC.002; New Mineral Binning Stats2.xls.

Table 6.11-12. Na Statistics for Mineral Clustering and Aqueous Binning

Na by Mineral Clustering (Moles/kg H ₂ O)					Na by Aqueous Binning (Moles/kg H ₂ O)				
Cluster	Waters (n)	Mean	Standard Deviation	% Coefficient of Variation	Bin	Waters (n)	Mean	Standard Deviation	% Coefficient of Variation
Cluster 1	4	6.94E+00	3.21E-01	4.62	Bin 1	5	1.41E+00	5.00E-01	35.51
Cluster 2	6	6.75E+00	1.94E-01	2.87	Bin 2	13	3.38E+00	4.13E-01	12.21
Cluster 3	80	7.58E+00	6.74E-01	8.89	Bin 3	12	4.24E+00	3.22E-01	7.60
Cluster 4	12	6.97E+00	2.52E-01	3.61	Bin 4	43	6.47E+00	1.69E+00	26.14
Cluster 5	32	7.44E+00	5.08E-01	6.83	Bin 5	27	6.28E+00	2.39E-01	3.80
Cluster 6	45	7.00E+00	1.19E+00	17.02	Bin 6	8	7.38E+00	1.52E+00	20.58
Cluster 7	24	7.00E+00	4.38E-01	6.25	Bin 7	25	6.97E+00	4.96E-01	7.12
Cluster 8	73	5.21E+00	2.10E+00	40.43	Bin 8	22	8.02E+00	9.77E-01	12.19
Cluster 9	36	6.95E+00	2.89E-01	4.16	Bin 9	58	7.82E+00	9.65E-01	12.35
Cluster 10	46	6.87E+00	9.80E-02	1.43	Bin 10	10	7.26E+00	4.34E-01	5.97
Cluster 11	10	8.60E+00	1.10E+00	12.84	Bin 11	145	7.08E+00	2.61E-01	3.69
Mean				9.90	Mean				13.38

Source: Output DTN: MO0310SPAPCEAC.002; New Mineral Binning Stats2.xls.

Table 6.11-13. S Statistics for Mineral Clustering and Aqueous Binning

S by Mineral Clustering (Moles/kg H ₂ O)					S by Aqueous Binning (Moles/kg H ₂ O)				
Cluster	Waters (n)	Mean	Standard Deviation	% Coefficient of Variation	Bin	Waters (n)	Mean	Standard Deviation	% Coefficient of Variation
Cluster 1	4	6.75E-01	3.00E-02	4.44	Bin 1	5	1.89E-03	1.27E-04	6.74
Cluster 2	6	7.49E-01	7.25E-02	9.67	Bin 2	13	1.90E-03	1.29E-04	6.80
Cluster 3	80	6.26E-01	9.53E-03	1.52	Bin 3	12	2.58E-03	1.76E-03	68.27
Cluster 4	12	8.53E-01	3.60E-02	4.22	Bin 4	43	3.84E-01	9.58E-02	24.93
Cluster 5	32	7.07E-01	8.02E-02	11.34	Bin 5	27	1.03E+00	2.83E-02	2.76
Cluster 6	45	9.64E-01	1.98E-01	20.57	Bin 6	8	8.59E-01	4.38E-02	5.10
Cluster 7	24	9.59E-01	1.97E-01	20.49	Bin 7	25	1.24E+00	1.17E-01	9.43
Cluster 8	73	2.27E-01	2.03E-01	89.31	Bin 8	22	1.62E+00	2.38E-01	14.65
Cluster 9	36	1.31E+00	2.31E-01	17.58	Bin 9	58	7.45E-01	1.07E-01	14.34
Cluster 10	46	7.79E-01	3.47E-02	4.45	Bin 10	10	1.16E+00	1.02E-01	8.77
Cluster 11	10	1.67E+00	3.47E-01	20.78	Bin 11	145	6.91E-01	7.68E-02	11.12
Mean				18.58	Mean				15.72

Source: Output DTN: MO0310SPAPCEAC.002; New Mineral Binning Stats2.xls.

Table 6.11-14. Si Statistics for Mineral Clustering and Aqueous Binning

Si by Mineral Clustering (Moles/kg H ₂ O)					Si by Aqueous Binning (Moles/kg H ₂ O)				
Cluster	Waters (n)	Mean	Standard Deviation	% Coefficient of Variation	Bin	Waters (n)	Mean	Standard Deviation	% Coefficient of Variation
Cluster 1	4	3.63E-02	2.00E-03	5.51	Bin 1	5	1.42E-03	1.86E-04	13.14
Cluster 2	6	1.30E-01	9.81E-02	75.67	Bin 2	13	2.26E-03	3.16E-04	13.97
Cluster 3	80	9.13E-02	4.71E-02	51.61	Bin 3	12	2.33E-03	5.22E-04	22.40
Cluster 4	12	1.18E-01	7.69E-02	65.12	Bin 4	43	3.49E-03	1.26E-03	35.96
Cluster 5	32	1.13E-01	4.84E-02	42.83	Bin 5	27	6.08E-03	3.95E-03	65.00
Cluster 6	45	4.61E-02	7.57E-02	164.06	Bin 6	8	7.71E-02	7.78E-02	100.86
Cluster 7	24	1.79E-02	7.77E-03	43.28	Bin 7	25	9.58E-03	4.00E-03	41.72
Cluster 8	73	2.94E-03	1.21E-03	41.25	Bin 8	22	4.16E-03	1.18E-03	28.36
Cluster 9	36	8.95E-03	5.51E-03	61.58	Bin 9	58	1.03E-01	7.03E-02	67.99
Cluster 10	46	1.12E-01	5.92E-02	52.71	Bin 10	10	1.07E-02	2.49E-03	23.16
Cluster 11	10	3.50E-03	1.04E-03	29.69	Bin 11	145	9.70E-02	5.56E-02	57.33
Mean				57.57	Mean				42.72

Source: Output DTN: MO0310SPAPCEAC.002; New Mineral Binning Stats2.xls.

6.11.2 Transport Affected Salt Assemblages

The environment on the surface of the drip shield or waste package is subject to thermal-hydrologic conditions that may involve splashing. The surface may be covered with dust and debris on the surface, and may have dents or depressions caused by rockfall. In addition, crevices may form as stress corrosion cracks or where debris contacts the surface, and these may harbor stagnant liquid or immobilized solid phases. Over the long term, the surface of the drip shield and the waste package (depending on local seepage and possible drip shield damage) is subject to cumulative evaporation amounting to hundreds to thousands of liters per waste package.

Interaction of seepage water with the surfaces of the drip shields or exposed waste packages may produce mineral precipitates because the surface temperature is greater than that of the host rock resulting in a lower local relative humidity. The most volumetrically important of these precipitates are calcite, anhydrite, and forms of silica (Section 6.13). The effect of these processes on the chemical environment for corrosion is the possible accumulation of separated salts as well as inert products that affect hydraulics and chemical heterogeneity (Hall and Walton, 2003 [DIRS 170586]). The effects of relatively inert scale (e.g., silica or calcite) are included in the measured data used to develop the corrosion models (BSC 2004 [DIRS 169984], Sections 1.2 and 6.4.4.2), however the effects from separation of potentially aggressive species such as chloride, are addressed explicitly in the seepage evaporation abstraction.

Soluble salts containing chloride may precipitate along flow pathways if the temperature and humidity conditions (e.g., on the drip shield or waste package) are sufficiently different from the conditions at the drift wall. If transport of the residual liquid phase occurs, the chloride-bearing precipitates are separated from the other chemical components of seepage, such as nitrate. The process could be enhanced by the presence of precipitates such as silica or calcite, which could cause ponding or channeling. Dents caused by rockfall or resulting from seismic shaking could cause similar effects on flow. Although this situation may be rare, it is incorporated in the seepage evaporation abstraction model used for TSPA in relation to the potential for localized corrosion of the waste package outer barrier. The drip shield titanium material is not susceptible to localized corrosion under in-drift environmental conditions (BSC 2004 [DIRS 169845], Section 6.3.3).

Halite Separation—The first mineral to alter chloride during evaporation of the seepage abstraction bin waters is halite (NaCl). The most cautious approach for modeling deleterious chloride separation is to consider at what point halite begins to precipitate, ignoring the concurrent transport issues. Examination of the seepage water lookup tables (output DTN: MO0304SPACSALT.000, *Evap_Look-up-Tables.zip*) shows in Figure 6.11-1 a range of relative humidity values dependant upon temperature and $p\text{CO}_2$.

For implementation in TSPA-LA a single cutoff value may be desirable. This bounding value has been determined from examination of two sources of halite precipitation relative humidity at various temperatures. These sources were the DTN: LL031106231032.007 ([DIRS 170605], *ExptDRHCalcsKracekRev00c.xls*) covering 20°C to 110°C, and “Humidity Fixed Points of Binary Saturated Aqueous Solutions” (Greenspan 1977 [DIRS 104945], Table 2) covering 20°C to 80°C. The highest relative humidity of these results comes from the report by Greenspan

(1977 [DIRS 104945]) at 80°C with 76.29 (± 0.65) percent. Given the slight uncertainty on this value, it has been rounded upwards to 77 percent. For complete data sets see the output DTN: SN0403T0503404.001.

Therefore, when seepage occurs directly on waste packages and the relative humidity on the waste package surface is less than 77%, separation of sodium chloride precipitate is allowed to occur and to initiate localized corrosion. This threshold relative humidity is higher than any value predicted for precipitation of sodium chloride in any of the seepage bins and is a bounding upper limit as determined by pure sodium chloride salt deliquescence experiments.

Source: Output DTN: SN0403T0510102.001.

NOTE: Each bin shows data at nine points for all three temperatures (40°C, 70°C, 100°C) and $p\text{CO}_2$ (10^{-4} , 10^{-3} , and 10^{-4} bars).

Figure 6.11-1. Relative Humidity at Initial Precipitation of Halite in Median Bin Waters.

6.11.3 Brine Compositions Due to Dust Deliquescence

In the P&CE model, the compositions of brines formed by dust deliquescence are estimated using the IDPS model and a Pitzer-based thermodynamic model generally applicable to bulk solutions. The model does not take into account the effects of surface interactions and interfacial forces, which are likely to be important in the case of dust deliquescence, where the brine volume can be very small, and the corresponding water:solid ratio is very large. Here, the possibility of using alternate conceptual models for modeling deliquescent brine compositions in the dust is examined.

The amounts of soluble anions in the dust (represented in the model by soluble salts) are small (Section 4.1.6), and the volume of brine that is likely to form by dust deliquescence is limited. In the calculated EQ3/6 dust leachate evaporation modeling runs described in Section 6.10, the

eutectic point is not reached until the amount of water remaining in the model system is around 10^{-5} kg, or about 10 μL (Figure 6.13-40). Thus, brines forming initially, by deliquescence at the system eutectic, will have a very small volume. Because water compositions in the calculated dust leachate modeling runs represent leachate from a 20-gram aliquot of dust, water:solid ratios in the dust will be on the order of 10 $\mu\text{L}/20$ g. (This typical amount of water is only that which is associated with crystals of the deliquescent salts, and does not include moisture that is adsorbed on the surfaces of dust grains or held in the micropores by capillarity. The latter occurrences of moisture are considered to have no effect on the corrosion environment).

At such low water:solid ratios, the brine exists in close proximity to the mineral grains of the dust, so that solid-liquid interface processes may be important. Water in close enough proximity to silicate mineral surfaces tends to be ordered by hydrogen bonding between the molecules and the surface, and has a lower activity than for bulk solution conditions. Capillary effects on the activity of the water may also be significant, depending on the geometry of brine droplets.

The effects previously described serve to lower the activity of water in the dust, without necessarily lowering the solute activities. Thus, the model may over predict the relative humidity at which particular equilibrium solution conditions occur.

Another concept not considered in this model is the potential for heterogeneity in the dust. The deliquescence calculations in Section 6.10 use homogeneously distributed soluble salt mineral phases in the dust, and presume that all phases are in contact with each other. These salt minerals constitute a minor fraction of the dust, and individual grains of salt minerals must be very small, for homogenous distribution. The grain size and distribution homogeneity of soluble salt minerals in the dust are not known, which allows the possibility for more chemical heterogeneity in the dust layer than is accommodated in the model.

Finally, in the EBS model for deliquescent brine evolution, brine composition is only a function of the RH and the starting composition. Corrosion reactions are neglected, or, equivalently, consume only water. As the minute volumes of brine are in equilibrium with the atmosphere, the supply of water is relatively infinite. Salt components in the brine are conserved (with respect to corrosion) and they are treated as catalysts rather than reactants. In actuality, some fraction of the salt components will be incorporated into the corrosion products, and, because the total mass of salts (and the volume of brine) is very small, the brine composition may change significantly with time, even at constant RH. This process may be important in limiting the amount of corrosion that could occur due to dust deliquescence, and is currently not implemented in the P&CE model.

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 169856]), 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 deliquescent 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 169856], 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)

- The various investigated model conceptualizations (vapor-pressure model, drift location, stratigraphic columns, open versus closed drift wall) (Table 6.6-1)
- Ranges of input parameters other than water composition (in this case infiltration rates and CO₂ diffusion coefficients) (Section 6.5.4).

The relative spread caused by the variability of input water compositions (computed as standard deviation) is shown as a function of time in Table 6.6-2. This spread is up to around one order of magnitude and in many cases much less. The spread overlaps with, and in most cases is larger than, the spread introduced by use of the different model conceptualizations and ranges of other input data considered (compare Figures 6.5-24a through 6.5-37a to Figures 6.5-24b through 6.5-37b). This is quantitatively demonstrated in Post-Processing Analysis for THC Seepage (BSC 2004 [DIRS 169858]).”

Section 8.1 Modeled Coupled Processes and Uncertainty, p. 8-2:

“These THC Seepage Model simulations covered a wide range of the most important uncertainties, and the range of results obtained is represented by the principal source of uncertainty, which is the natural variability in input water composition. In the spread of simulation results corresponding to the range of input water composition, the uncertainties in predicted concentrations of aqueous species and of CO₂ gas are estimated to approximately one order of magnitude or less (Section 6.6.2).”

6.12.2 Uncertainties in the In-Drift Precipitates/Salts Model That Affect Characterization and Binning of Seepage Water Compositions

The IDPS model is used to predict the changing compositions of potential seepage waters as they evaporatively evolve to concentrated brines (BSC 2004 [DIRS 169863], Section 1). The output of this model is a set of lookup tables that describe the chemical compositions of these waters as a function of relative humidity. As relative humidity decreases, the degree of evaporation increases, which in turn causes an increase in the salinities of these waters. The lowest relative humidity predicted by the model corresponds to the deliquescence point (*DRH*) of the water at the specified temperature and fugacity of carbon dioxide. At relative humidity values below this deliquescence point, the brine is no longer stable and only dry salts remain. The output parameters used in TSPA-LA are pH, ionic strength (*I*), *DRH*, the total concentrations of chloride and nitrate, and the Cl:NO₃ ratio. The uncertainty in the values of these output parameters due to model uncertainty is addressed in this section. Model uncertainties result from uncertainties in the conceptual model, model equations, the choice of mineral suppressions, and constraints in the thermodynamic database.

The uncertainty that is readily quantifiable and useful to the TSPA-LA is the uncertainty in the EBS Physical and Chemical Environment model output parameter values for pH, ionic strength, *DRH*, the total concentrations of chloride and nitrate, and the Cl:NO₃ ratio. The IDPS model uncertainty contributes to this, and is determined by comparing IDPS model evaporation predictions to experimentally measured data.

The overall IDPS model uncertainty in these outputs is quantified in *In-Drift Precipitates/Salts Model* (BSC 2004 [DIRS 169863], Section 7.5) and is presented in Table 6.12-1.

The uncertainty values for *I* and *Cl* are in units of log molal, whereas for the ratio *Cl:NO₃* the error is for the log of the molal ratio and is therefore unitless. The units for pH and *DRH* are their native pH units and native percent *RH* units, respectively. It is noted that *Cl*, *NO₃* and *Cl:NO₃* are not independent parameters and only two of these three must be passed to the TSPA-LA.

Table 6.12-1. Estimated Model Uncertainty Ranges for In-Drift Precipitates/Salts Model Outputs

Parameter	Units	RH Range 100% to 85%	RH Range 85% to 65%	RH Range 65% to 60%	RH Range 60% to 40%	RH Range 40% to 0%
pH	pH units	± 1	± 1	± 1	± 2	± 2
Ionic Strength	log molal	± 0.1	not used ^a	not used ^a	not used ^a	not used ^a
Cl	log molal	± 0.0	± 0.2	± 0.5	± 0.7	± 0.7
Cl:NO ₃	log molal ratio	± 0.0	± 0.2	± 0.5	± 0.7	± 1
DRH	%RH units	± 5	± 10	± 10	± 10 ^b	± 15 ^c

Source: DTN: MO0312SPAESMUN.002 [DIRS 166329].

NOTES: These uncertainties are defined as uniform distributions encompassing ~95 percent probability. Uncertainties between 85 percent RH and 40 percent RH are based primarily on ternary systems involving Na, K, and Ca. Uncertainties below 40 percent are primarily based on binary and ternary systems involving Mg and Ca.

^a Prediction of ionic strength is for colloids model. At RH<85 percent, ionic strength exceeds 3 molal, which is far above the critical ionic strength where colloids are stable.

^b Exceptions:

1. Predicted DRH for Ca(NO₃)₂ is 20 to 25 percent RH units higher than data: error not conservative.
2. Predictions likely more than 10 percent RH too high for Mg(NO₃)₂ at T>100°C: error not conservative.

^c Exceptions:

1. Predicted DRH for Ca(NO₃)₂ is 20 to 25 percent RH units higher than data.

6.12.3 Discretization Error Associated with Binning Abstractions

This section examines the uncertainty tied to the binning abstractions for THC seepage (Section 6.12.3.1) and dust leachate (Section 6.12.3.2), where the variability in each of the bins is considered to quantify the largest amount of uncertainty possible within a bin during the evaporative process. The variability is examined at four different relative humidity (or activity of water) conditions: unevaporated, 98 percent, 85 percent, and 65 percent. These four snapshot modeling points represent locations that capture the effects of major chemical divides that may occur, such as the precipitation of calcite and halite. At the four locations along the evaporative pathway, the objective is to see where the variability is greatest within the bin. The largest amount of variability along this pathway is the uncertainty that can be applied to any given parameter on THC seepage or dust leachate chemistry lookup tables. The probability distribution for the within-bin uncertainty is defined to be log-uniform. This designation is conservative because the probability of realizing an extreme value is higher than it is for triangular or normal distributions. A uniform distribution is also generally apparent from Figures 6.6-9 through 6.6-19.

6.12.3.1 THC Seepage Lookup Tables

The bin histories for each water (Tables 6.6-8 through 6.6-12) were mapped back to the five unevaporated THC seepage model time history chemistries (Table 6.6-1) in *New Non Evaporated Binning Statistics02.xls*, which is archived in DTN: MO0310SPAEBSEUE.002. The standard functions of Excel (median, minimum, maximum, standard deviation(s), and 2s (where s is multiplied by 2)) were used to calculate the statistics. This is done to determine the variability within the bins before the chemistries were evaporated. The variability of the unevaporated waters was not included in estimates of binning variability because it decreases rapidly as the waters are "normalized" by even small degrees of evaporation.

For the 98 percent and 85 percent relative humidity conditions, *Checked 98% RH EBS THC Seepage Binning Abstraction REV03.xls* and *Checked 85% RH EBS THC Seepage Binning Abstraction REV03.xls* were developed to show the variability of seepage water chemistry due to evaporation to brine water activities corresponding to 98 and 85 percent RH. These spreadsheets and associated EQ6 input and output files are archived in DTN: MO0310SPAEBSSB.002. Recalculating the EQ6 input files listed in Table 6.6-1 at 98 percent and 85 percent relative humidity generates the EQ6 input files used in this calculation. GETEQData software was used to extract the final equilibration results from each output file. Standard Excel functions (median, minimum, maximum, standard deviation(s), and 2s) are used to calculate the statistics to determine the variability within the bins after the chemistries were evaporated. The extracted output variables, found on the "Data & Plots" worksheet in both spreadsheets, include pH, activity of water ($a_w \approx 0.98$ or 0.85), ionic strength (I), and total molalities of the aqueous constituents (Al, C, Ca, Cl, F, K, Mg, N, Na, S, and Si). The waters in the "Data & Plots" worksheet are sorted by bin and the chemistries for each of the 11 bins were copied and pasted into separate abstraction bin worksheets. Two standard deviations (2s) are considered reasonable for an estimate of the 95 percent distribution about the mean for normally distributed chemistries. These variability distributions were not used in the calculations below because the values are log normally distributed.

These spreadsheets along with the binning spreadsheet (DTN: MO0310SPAEBSCB.003, *Final Checked EBS THC Seepage Binning Abstraction REV 4.xls*) documented in Section 6.6.4 were then used as input into a new set of spreadsheets where the parameter data was log transformed so that the statistics would be log normally distributed. These spreadsheets are listed in Table 6.12-2. Within each spreadsheet, statistics for the log-transformed data can be referenced.

Table 6.12-2 Spreadsheets Containing Log Transformed Data and Statistics for Each of the Uncertainty RH Locations Evaluated

RH Location	Spreadsheet Name
98%	<i>Checked 98% RH EBS THC Seepage Binning Abstraction REV03 log transform.xls</i>
85%	<i>Checked 85% RH EBS THC Seepage Binning Abstraction REV03 Log transform.xls</i>
65%	<i>Final Checked EBS THC Seepage Binning Abstraction REV 4 log transform.xls</i>

Source: Output DTN: MO0310SPAPCELT.000.

A review of the 65 percent RH data indicated that in many instances the uncertainty values were skewed because the evaporative evolution had passed beyond the halite divide, causing larger uncertainty than should be present for the uncertainty caused by bin or lookup table variability.

Therefore, only the data from 98 and 85 percent RH were used to develop Tables 6.12-3 and 6.12-4. Table 6.12-3 provides the relative humidity location (e.g., 98 or 85 percent RH) with the most uncertainty (largest 2s value). Only the uncertainties for the parameters of interest to the TSPA-LA are presented in the following tables; uncertainties for all other species of interest can be found in the spreadsheets listed in Table 6.12-2. Ionic strength is not included in this table as its uncertainty is only considered at 98 percent RH (ionic strength is above 1 M at this RH). This is because the ionic strength values (I) will only be utilized by the TSPA-LA when I is less than 1 M (e.g., for colloid stability modeling, the colloids are unstable when $I > 0.05$ M) (BSC 2004 [DIRS 170025], Section 6.3.1 and Table 6-12).

Table 6.12-3. Relative Humidity Point with the Most Variability for Bins 1 through 11 for pH, Cl, and Cl:NO₃

Species	Bin 1	Bin 2	Bin 3	Bin 4	Bin 5	Bin 6	Bin 7	Bin 8	Bin 9	Bin 10	Bin 11
pH	85	98	85	85	85	98	85	98	98	85	85
Cl	98	98	98	98	98	98	98	98	98	85	98
Cl:NO ₃ *	85/98	85/98	85/98	85/98	85/98	85/98	85/98	85/98	85/98	85/98	85/98

NOTES: Ionic strength was only considered at the 98 percent RH level.

*Cl:NO₃ ratio is the same for 85 percent and 98 percent RH.

Given the 2s statistics presented in the spreadsheets on Table 6.12-2 and the RH location where the most variability lies (Table 6.12-3), Table 6.12-4 has been developed to give the uncertainty that can be applied to any given discrete parameter used in the TSPA-LA.

Table 6.12-4. The Error Applied to the THC Seepage Lookup Tables for pH, I, Cl, and Cl:NO₃ Based on the RH with the Highest Variability in Bins 1 through 11 (Errors are Based on 2s Values)

Species	Bin 1	Bin 2	Bin 3	Bin 4	Bin 5	Bin 6	Bin 7	Bin 8	Bin 9	Bin 10	Bin 11
±pH	0.13	0.25	0.42	0.65	0.49	0.77	0.28	0.33	0.46	0.12	1.05
±Log I*	0.04	0.06	0.03	0.08	0.07	0.11	0.04	0.04	0.07	0.03	0.05
±Log Cl	0.13	0.10	0.03	0.30	0.13	0.17	0.48	0.50	0.38	0.11	0.43
±Log Cl:NO ₃	0.92	0.67	0.43	1.10	0.57	0.97	0.56	0.73	0.53	0.75	0.32

Source: Output DTN: MO0311SPAEP MUT.000.

NOTE: *Based on 98 percent RH results only.

The usage of uncertainty on the log of Cl:NO₃ is implemented in order to account for correlation between these two species. This is done rather than passing along an independent nitrate uncertainty value that is not related to the variability in chloride. One of the strongest correlations exists in Bin 9 at 98 percent, where the log nitrate uncertainty 2s value is 0.72 (from calculations within output DTN MO0310SPAPCELT.000) compared to the log Cl:NO₃ 2s value of 0.53 (Table 6.12-4). This is a way to implement correlation because, for example, if the chloride value goes to an extreme value low (−0.38 for Bin 9), the nitrate will not be able to go outside of the log Cl:NO₃ range (maximum of +0.53). Whereas, using nitrate uncertainty instead could result in an extreme log Cl:NO₃ ratio difference of 1.10 (log NO₃ 2s value of 0.72 plus log Cl of 0.38). Section 6.12.5.3 provides specific TSPA-LA implementation instructions.

6.12.3.2 Dust Leachate Lookup Tables

The statistical data for the 98 percent and 85 percent RH are calculated in a similar manner to the calculations performed in Section 6.12.3.1. Table 6.12-5 lists the spreadsheets and DTN for the EQ6 files that are used to develop the tables. For the unevaporated spreadsheet, the EQ6 output files that are generated for the 65 percent RH condition are also used.

Table 6.12-5. Dust Leachate Variability Calculations at 85 and 98 Percent RH

RH location	Excel File	Location of EQ6 input and output Files
98%	<i>EBS Dust Leachate 98% RH uncert anal.xls</i>	DTN: SN0310T0510102.010, directory /98rh
85%	<i>EBS Dust Leachate 85% RH uncert anal.xls</i>	DTN: SN0310T0510102.010, directory /85rh

Source: Output DTN: MO0310SPADLBU4.001.

Two of these spreadsheets along with the binning spreadsheet (EBS Dust Leachate Binning Abstraction Rev 01.xls) documented in Section 6.10.5.2 are then used as input into a new set of spreadsheets where the statistics are applied to the log-transformed parameter data. These spreadsheets are listed on Table 6.12-6. Within each spreadsheet, statistics for the log-transformed data can be referenced.

Table 6.12-6. Spreadsheets Containing Log Transformed Data and Statistics for Each of the RH Locations Evaluated for Uncertainty

RH Location	Spreadsheet Name
98%	<i>EBS Dust Leachate 98% RH uncert anal log transform.xls</i>
85%	<i>EBS Dust Leachate 85% RH uncert anal log transform.xls</i>
65%	<i>EBS Dust Leachate Binning Abstraction Rev 01 log transform.xls</i>

Source: Output DTN: MO0310SPAPCELT.000.

As with the seepage waters, a review of the 65 percent RH data indicated that in many instances the evaporative evolution had passed beyond the halite divide, causing larger uncertainty than should be present for the uncertainty caused by bin or lookup table variability. Therefore, only the data from 98 and 85 percent RH were used to develop Tables 6.12-7 and 6.12-8. Table 6.12-7 lists the relative humidity with the most uncertainty within the bins. Table 6.12-8 presents only the uncertainties for the parameters of interest to the TSPA-LA; uncertainties for all other species of interest can be found in the spreadsheets listed in Table 6.12-6.

Table 6.12-7. Table Giving the Relative Humidity with the Most Uncertainty in Bins 1 through 5 for pH, Cl, and Cl:NO₃

Species	Bin 1	Bin 2	Bin 3	Bin 4	Bin 5
pH	85	85	98	85	85
Cl	85	85	98	98	98
Cl:NO ₃	98	98	85	85	85

NOTE: Bin 6 has no lookup table uncertainty.

The median and 2s statistics presented in the spreadsheets listed in Table 6.12-6 and the RH condition for which the most variability occurs (Table 6.12-7) were used to develop

Table 6.12-8, which gives the uncertainty that can be applied to any given discrete parameter used in the TSPA-LA.

Table 6.12-8. The Error Applied to the Dust Leachate Lookup Tables for pH, I, Cl, and Cl:NO₃, Based on the RH with the Highest Uncertainty within Bins 1 through 5 (Errors are Based on 2s Values)

Species	Bin 1	Bin 2	Bin 3	Bin 4	Bin 5
±pH	0.44	0.10	0.38	0.19	0.25
±Log I*	0.03	0.07	0.06	0.04	0.05
±Log Cl	0.16	0.19	0.27	0.19	0.21
±Log Cl:NO ₃	0.23	0.28	0.33	0.35	0.44

Source: Output DTN: MO0311SPAEP MUT.000.

NOTES: Bin 6 has no lookup table uncertainty.

*Based on 98 percent RH results only.

6.12.4 Factors Showing No Significant Impact on Water Chemistry

Several potential sources of perturbation to the predicted water chemistries contained within the lookup tables have been evaluated in sensitivity studies. These include:

- Degradation of stainless steel in the ground support material
- Inclusion of bromide in the seepage water compositions
- Lookup table extrapolation as a function of $p\text{CO}_2$
- Use of alternate mineral suppressions.

Analyses performed on the first two of these sources demonstrate that there is no increase in overall model uncertainty, except in the case where Cr(VI) is designated as the stable chromium oxidation state. For $p\text{CO}_2$, it is shown that extrapolation outside the lookup table values ($p\text{CO}_2$ at 10^{-2} , 10^{-3} , and 10^{-4} bar) is valid within the modeling error, with the only significant effect upon pH being ~0.15 pH units at $p\text{CO}_2 = 2 \times 10^{-2}$ bar, which is the highest $p\text{CO}_2$ found in the lookup tables. Alternate mineral suppressions are also examined, and in general are found to have no significant effect upon lookup table values, with the largest deviation being ~0.2 pH units.

These studies show that variations due to these factors fall well within the model uncertainty ranges and demonstrate that any additional errors caused by their exclusion from the lookup table calculations are subsumed by other modeling uncertainties (see Section 6.12.5.2 for uncertainty values determined for the TSPA-LA lookup tables).

For the calculations produced in this section, two general base cases are selected. This is done to characterize the uncertainty that is possible within the preceding model calculations. These cases represent the most likely (based on actual number of data points available) seepage water bin (Bin 11 in Table 6.6-6) and the most likely dust leachate water bin (Bin 5 in Table 6.10-7). The base-case files are listed on Table 6.12-9.

Table 6.12-9. Base-Case EQ3/6 Input Files for Uncertainty Analysis

Seepage Water Bin 11EQ3 input File	Seepage Water Bin 11EQ6 input File	Dust Leachate Water Bin 5 EQ3 input File	Dust Leachate Water Bin 5 EQ6 input File
<i>bin11.3i</i>	<i>11c3t7e.6i</i>	<i>p26_25b.3i</i>	<i>d5c3t07.6i</i>
Source: Output DTN: MO0304MWDSAB11.001	Source: Output DTN: MO0304MWDEBSSA.000	Source: Output DTN: SN0310T0510102.010	Source: Output DTN: SN0310T0510102.011

6.12.4.1 Degradation of Stainless Steel in Ground Support Components

A range of possible sources of uncertainty in the abstracted seepage-ground support interactions for Stainless Steel Type 316L is examined here. All but one was found to have no effect on the values of the lookup table results, with all deviations less than 0.04 for pH and 0.01 molal for ionic strength. Usage of Cr(VI) resulted in a large drop in pH (to 2.7 unevaporated) and increased ionic strength by 0.56 molal when evaporated. Comparisons are primarily made to the base-case scenario of evaporated seepage waters, whose files are labeled as "Run" number 2 in Table 6.8-2. Some of the uncertainty cases required their own "base-case" calculation run for comparative purposes, included in Sections 6.12.4.1.3 through 6.12.4.1.4, as there are changes in their basic chemical parameters (e.g., $p\text{CO}_2$).

All calculation runs utilized a modified *Data0.YMP.R2* thermodynamic database as was described in Section 6.8.3; this modification is contained within DTN: SN0312T0510102.013 in filename *Cr-database.zip*.

6.12.4.1.1 Alternate Corrosion Rates

A sensitivity analysis has been performed with a corrosion rate ten times greater than the base-case value. This higher corrosion rate is investigated to evaluate the base-case model results and determine the effect upon seepage water chemistries. This analysis is implemented by increasing the abstracted Stainless Steel Type 316L species dissolved into the Bin 11 crown seepage water by a factor of ten, resulting in the addition of 4.7×10^{-2} moles of Stainless Steel Type 316L. Table 6.12-10 shows the EQ6 input/output files generated for this uncertainty case. The bottom half of the pickup file from *ssbin11.6p* is used as the bottom half of the subsequent *ssbin11e.6i* evaporation run.

Table 6.12-10. EQ6 Input/Output Files for Stainless Steel Type 316L Corrosion Rate Uncertainty Case

Input File Names	Output File Names	Pickup File Names
<i>SSBin11.6i</i>	<i>ssbin11.6o</i>	<i>ssbin11.6p</i>
<i>ssbin11e.6i</i>	<i>ssbin11e.6o</i>	—

Source: Output DTN: SN0312T0510102.013, *Uncertainties.zip*.

NOTE: These files are in directory: \Cor Rate.

The calculated results of this uncertainty run are compared with the bounding base-case model; the results are summarized in Table 6.12-11. There is no calculable difference in the aqueous water chemistry.

Table 6.12-11. Comparison of pH and Ionic Strength for Corrosion Rate Uncertainty Case

RH	Uncertainty Case		Base Case		Difference	
	pH	I (molality)	pH	I (molality)	pH	I (molality)
100	7.880	0.00606	7.879	0.00605	0.001	0.00001
98	9.462	0.7313	9.462	0.7312	0.000	0.0001

Source: Output DTN: SN0312T0510102.013, *Uncertainties.zip*, *UncertaintyCases.xls*, sheet Corrosion Rate.

6.12.4.1.2 Cr(VI)

A sensitivity analysis is performed to examine the impact on seepage water chemistry resulting from the formation of Cr(VI), which could occur under extremely oxidizing conditions. As this case requires a completely new speciation from that of the base case, an EQ3NR calculation run is required and its pickup file is used as the bottom half of the calculated EQ6 Stainless Steel Type 316L dissolution run. Also, the bottom half of the pickup file from *ssbin11.6p* is used as the bottom half of the subsequent calculated *ssbin11e.6i* evaporation run. Table 6.12-12 contains the EQ3/6 filenames for this uncertainty case.

Table 6.12-12. EQ3/6 Input/Output Files for Stainless Steel Type 316L Cr(VI) Uncertainty Case

Input File Names	Output File Names	Pickup File Names
<i>bin11.3i</i>	<i>bin11.3o</i>	<i>bin11.3p</i>
<i>SSBin11.6i</i>	<i>ssbin11.6o</i>	<i>ssbin11.6p</i>
<i>ssbin11e.6i</i>	<i>ssbin11e.6o</i>	—

Source: Output DTN: SN0312T0510102.013, *Uncertainties.zip*.

NOTE: These files are in directory: \Cr(VI).

The results of this uncertainty run are also compared with the bounding base case and are summarized in Table 6.12-13. Unlike the other stainless steel sensitivity cases, dramatic changes are seen in the predicted pH and ionic strength. This is directly due to the production of five protons for every Cr(III) converted to Cr(VI)O_4^{2-} , which exceeds the acid neutralizing capacity of the seepage water from $\text{CO}_{2(g)}$ buffering. As discussed in Section 6.8.3.1, it is unlikely that Cr(VI) will significantly contribute to the in-drift chemical environment.

Table 6.12-13. Comparison of pH and Ionic Strength for Cr(VI) Uncertainty Case

RH	Uncertainty Case		Base Case		Difference	
	pH	I (molality)	PH	I (molality)	pH	I (molality)
100	2.7281	0.00922	7.879	0.00605	-5.1509	0.00317
98	1.7107	1.28679	9.462	0.7312	-7.7514	0.5556

Source: Output DTN: SN0312T0510102.013, *Uncertainties.zip*, *UncertaintyCases.xls*, sheet Cr(VI).

6.12.4.1.3 Bin 07 Seepage

Another crown seepage abstracted water has been examined to determine whether a different starting water chemistry would affect the Stainless Steel Type 316L interactions. Bin 07 (DTN: MO0304MWDSAB11.001) was chosen, because it represents seepage water that is

likely to enter the repository during relatively long periods (i.e., 10,000 years, Tables 6.6-8 through 6.6-12), thus being appropriate given the potentially long lifetimes of stainless steel.

The EQ3/6 input, output and pickup files are listed in Table 6.12-14. Because a different starting water composition is used, the EQ3NR speciation was redone by replacing the water chemistry description in file *Bin 11.3i* (Section 6.8.4.1) with the descriptions residing in Bin 07. The rest of the procedure is identical to that used for the base-case calculation runs described in Section 6.8.4.1.

Table 6.12-14. EQ3/6 Input/Output Files for Stainless Steel Type 316L Bin 07 Uncertainty Case

Input File Names	Output File Names	Pickup File Names
<i>Bin07.3i</i>	<i>in07.3o</i>	<i>bin07.3p</i>
<i>Bin07e.6i</i>	<i>bin07e.6o</i>	<i>bin07e.6p</i>
<i>SSBin07.6i</i>	<i>ssbin07.6o</i>	<i>ssbin07.6p</i>
<i>ssbin07E.6i</i>	<i>ssbin07E.6o</i>	—

Source: Output DTN: SN0312T0510102.013, *Uncertainties.zip*.

NOTE: These files are in directory: \Bin 7.

The results of this uncertainty calculation run are compared with the pure Bin 07 seepage water evaporation results; these results are summarized in Table 6.12-15. As with the base-case Bin 11 seepage water, there is effectively no change in the aqueous water chemistry caused by stainless steel corrosion and corrosion product formation in this case.

Table 6.12-15. Comparison of pH and Ionic Strength for Bin 07 Uncertainty Case

RH	Uncertainty Case		Base Case		Difference	
	pH	I (molality)	pH	I (molality)	pH	I (molality)
100	8.240	0.0110	8.240	0.0110	0.000	0.0000
98	9.520	0.7283	9.520	0.7284	0.000	-0.0001

Source: Output DTN: SN0312T0510102.013, *Uncertainties.zip*, *UncertaintyCases.xls*, sheet Bin 07.

6.12.4.1.4 CO₂ Fugacities

Two additional fugacities for CO₂ gas are examined as uncertainty cases; these are taken at 10⁻² and 10⁻⁴ bar. These fugacity uncertainty calculation runs are compared to the pure Bin 11 water chemistry results calculated at the same CO₂ fugacities.

The EQ3/6 input, output and pickup files are listed in Table 6.12-16 for the uncertainty case. As a different starting water fugacity of CO₂ is used, the EQ3NR speciation is redone and the resulting pickup file *bin11.3p* is fed to the bottom half of the two EQ6 calculation runs: *Bin11e.6i* and *SSBin11.6i* for the pure Bin 11 evaporation and SS316L/Bin 11 mixing calculation runs, respectively. The bottom half of the pickup file *ssbin11.6p* is used by the evaporation EQ6 calculation run, *ssbin11E.6i*.

Table 6.12-16. EQ3/6 Input/Output Files for Stainless Steel Type 316L $p\text{CO}_2 = 10^{-2}$ Uncertainty Case

Input File Names	Output File Names	Pickup File Names
<i>Bin11.3i</i>	<i>bin11.3o</i>	<i>bin11.3p</i>
<i>Bin11e.6i</i>	<i>bin11e.6o</i>	<i>bin11e.6p</i>
<i>SSBin11.6i</i>	<i>ssbin11.6o</i>	<i>ssbin11.6p</i>
<i>ssbin11E.6i</i>	<i>ssbin11e.6o</i>	—

Source: Output DTN: SN0312T0510102.013.

NOTE: These files are in directory: \PCO2 -2.

The results of the fugacity uncertainty calculation run at 10^{-2} bar are compared with the evaporation of pure Bin 11 water results at the same CO_2 fugacity, summarized in Table 6.12-17. There is no significant change in the predicted water chemistry caused by stainless steel corrosion and corrosion product formation at this higher CO_2 fugacity.

Table 6.12-17. Comparison of pH and Ionic Strength for $p\text{CO}_2 = 10^{-2}$ Uncertainty Case

RH	Uncertainty Case		Base Case		Difference	
	pH	I (molality)	pH	I (molality)	Ph	I (molality)
100	6.898	0.00606	6.898	0.00605	0.000	0.00000
98	8.741	0.7015	8.741	0.7012	0.000	0.0003

Source: Output DTN: SN0312T0510102.013, *Uncertainties.zip*, *UncertaintyCases.xls*, sheet "PCO2=-2."

The EQ3/6 input, output, and pickup files for the case with the CO_2 fugacity set at 10^{-4} bar are listed in Table 6.12-18. Because a different starting fugacity of CO_2 is used, the EQ3NR speciation was redone and the resulting pickup file *bin11.3p* was fed to the bottom half of the two EQ6 calculation runs: *Bin11e.6i* and *SSBin11.6i* for the pure Bin 11 evaporation and SS316L/Bin 11 mixing calculation runs, respectively. Again, the bottom half of the pickup file *ssbin11.6p* is used by the evaporation EQ6 calculation run, *ssbin11E.6i*.

Table 6.12-18. EQ3/6 Input/Output Files for Stainless Steel Type 316 $p\text{CO}_2 = 10^{-4}$ Uncertainty Case

Input File Names	Output File Names	Pickup File Names
<i>Bin11.3i</i>	<i>bin11.3o</i>	<i>bin11.3p</i>
<i>Bin11e.6i</i>	<i>bin11e.6o</i>	<i>bin11e.6p</i>
<i>SSBin11.6i</i>	<i>ssbin11.6o</i>	<i>ssbin11.6p</i>
<i>ssbin11E.6i</i>	<i>ssbin11e.6o</i>	—

Source: Output DTN: SN0312T0510102.013, *Uncertainties.zip*.

NOTE: These files are in directory: \PCO2 -4.

The results of this fugacity uncertainty calculation run at 10^{-4} are compared with the pure Bin 11 seepage water evaporation results at the same CO_2 fugacity; these are summarized in Table 6.12-19. There is no significant change in the water chemistry caused by stainless steel corrosion and corrosion product formation at this lower CO_2 fugacity.

Table 6.12-19. Comparison of pH and Ionic Strength for $p\text{CO}_2 = 10^{-4}$ Uncertainty Case

RH	Uncertainty Case		Base Case		Difference	
	pH	I (molality)	pH	I (molality)	pH	I (molality)
100	8.726	0.00600	8.726	0.00600	0.000	0.00000
98	9.957	0.7088	9.957	0.7089	0.000	-0.0002

Source: Output DTN: SN0312T0510102.013, *Uncertainties.zip*, *UncertaintyCases.xls*, sheet "PCO2=-4."

6.12.4.2 Evaporative Concentration of Br

The starting porewater compositions provided by the USGS (DTN: GS020408312272.003 [DIRS 160899]), which are used as primary inputs into the THC seepage model abstracted in Section 6.6, give trace quantities of many chemical components including Br^- . Bromide is a halide species that behaves conservatively in aqueous solutions, much like Cl^- , and will tend to concentrate in solution upon evaporation. Because total aqueous Br^- is not a modeled species in the THC seepage model, no direct model output for Br^- concentration is available. However, because halides are of concern to corrosion modeling, it is important to know to what level it would concentrate if present in the initial water. This sensitivity study investigates the evaporative concentration of Br^- in seepage waters and in dust leachate waters. The results show that the concentration of Br^- is small compared to the total halide concentrations in both water types. Therefore, the seepage and leachate compositions as presented in the lookup tables are adequate for the present applications.

6.12.4.2.1 Conceptual Framework

The calculation presented here compares the evaporative concentration of Br^- as a function of the Cl:Br ratio in the starting porewater compositions to the base-case THC seepage bin file listed in Table 6.12-9.

6.12.4.2.2 Calculation Set Up

Three bounding evaporation cases are developed by altering the seepage water base-case EQ3 input file (*bin11.3i*; see Table 6.12-9) through the addition of Br to the starting water composition. The Cl:Br ratio is calculated for samples collected at locations along the drift, as shown in Table 6.12-20 (from DTN: GS020408312272.003 [DIRS 160899]).

The concentration of Cl in each sample is divided by the value of Br (both in units of mg/L) to obtain the Cl:Br ratio. For concentrations of Br below the detection limit, the value of Br used for the calculation is one half of the detection limit and is indicated in the column labeled "Br mg/L^a." From the ratios calculated, the mean, maximum, and minimum values are obtained using the built-in functions in Excel from *Cl_BrREV2.xls* (Table 6.12-21).

The ratios found from this calculation are then used to calculate the amount of bromide to be added to the base-case 3i file (*bin11.3i*; Table 6.12-9). By dividing the chloride constraint value in bin11 (1.30×10^{-3} mol) from the base-case 3i file (*bin11.3i*; Table 6.12-9) by the Cl:Br ratio, as calculated in *Cl_BrREV2.xls*, three bromide concentrations are obtained as presented in Table 6.12-22.

Each Br value found in Table 6.12-22 is then inserted into the base-case EQ3 input file and run in EQ3 using the *Data0.ypf* database file, generating the EQ3 input and output files listed in Table 6.12-23. Once the new values for Br are added to the three 3i files, they are run using EQ3 v8.0. The pickup files replaced the bottom half of the base-case 6i file. Then, the 6i files are run at three temperatures (40°C, 70°C, and 100°C) using EQ6 v8.0 to obtain the final results of the alternate evaporation reaction. Lookup tables are generated using GETEQDATA to compare the results of the three Br-added evaporation runs to the base case.

Table 6.12-20. Cl and Br Data for Porewaters Collected in the Enhanced Characterization of the Repository Block

	Local Sample Name	SPC Number	Cl mg/L	Br mg/L	Br mg/L ^a	Cl:Br ratio
1	ECRB-SYS-CS400/3.8-4.3/UC	SPC00554610	29	<1	0.5	58
2	ECRB-SYS-CS400/5.6-6.2/UC	SPC00554611	21	<1	0.5	42
3	ECRB-SYS-CS600/3.6-4.0/UC	SPC00554612	22	<1	0.5	44
4	ECRB-SYS-CS1000/7.3-7.7/UC	SPC00554613	21	<1	0.5	42
5	ECRB-SYS-CS750/6.2-6.5/UC	SPC00554614	73	<1	0.5	146
6	ECRB-SYS-CS2150/5.5-6.1/UC	SPC00554615	27	<0.2	0.1	270
7	ECRB-SYS-CS900/5.4-5.9/UC	SPC00554616	37	<0.2	0.1	370
8	ECRB-SYS-CS850/5.1-5.6/UC	SPC00554617	32	<0.2	0.1	320
9	SD-9/990.4-991.7/UC	SPC00554618	23	<0.2	0.1	230
10	ECRB-SYS-CS900/3.5-4.1/UC	SPC00554619	53	0.3	0.3	177
11	ECRB-SYS-CS1000/12.9-14.0/UC	SPC00554620	22	<0.1	0.05	440
12	ECRB-SYS-CS450/5.3-6.0/UC	SPC00554621	66	0.4	0.4	165
13	ECRB-SYS-CS2300/4.3-4.9/UC	SPC00554622	23	<0.1	0.05	460
14	ECRB-SYS-CS500/12.0-16.7/UC	SPC00554800	54	0.4	0.4	135
15	ECRB-SYS-CS2000/16.5-21.1/UC	SPC00554801	26	<0.2	0.1	260
16	ECRB-SYS-CS2000/16.3-16.5/UC	SPC00554802	24	<0.2	0.1	240
17	ECRB-SYS-CS950/5.2-5.3/UC	SPC00554803	19	<0.2	0.1	190
18	ECRB-SYS-CS950/4.8-5.5/UC	SPC00554804	30	<0.2	0.1	300
19	SD-9/991.7-992.1/UC	SPC00554805	26	0.1	0.1	260
20	ECRB-SYS-CS1250/5.0-5.7/UC	SPC00554806	50	0.2	0.2	250
21	ECRB-SYS-CS1250/3.4-4.0/UC	SPC00554807	25	M	-	-
22	SD-9/670.5-670.6/UC	SPC00554808	46	0.3	0.3	153
23	ECRB-SYS-CS800/4.9-5.6/UC	SPC00554809	20	M	-	-
24	ECRB-SYS-CS700/5.5-5.8/UC	SPC00554810	64	<0.1	0.05	1280
25	NRG-7/7A/839.3-839.8/UC	SPC00554811	31	0.1	0.1	310

Source: DTN: GS020408312272.003 [DIRS 160899].

NOTE: M indicates not measured.

^a The value of bromide actually used for further analysis.

Table 6.12-21. Mean, Minimum, and Maximum Cl:Br ratios Present in Drift Samples

Parameter	Cl:Br
Avg	267
Min	42
Max	1280

Source: Output DTN: MO0310SPAPCEUA.002, *SeepageBrSensitivityStudy.zip*, in *Cl_BrREV2.xls*.

Table 6.12-22. Bromide Values Used as Input into EQ3 Input Files

Parameter	Bromide Constraint Value (molal)
Median	4.87E-06
Low	1.02E-06
High	3.10E-05

Source: Output DTN: MO0310SPAPCEUA.002.

Table 6.12-23. Br Uncertainty Analysis EQ3/6 Input and Output Files

File Type	High Br	Median Br	Low Br
EQ3 input File Name	<i>B11Mxbr.3i</i>	<i>B11Avgbr.3i</i>	<i>B11Mnbr.3i</i>
EQ3 Output File Name	<i>b11mxbr.3o</i>	<i>B11avgbr.3o</i>	<i>b11mnbr.3o</i>
Pick Up File Name	<i>b11mxbr.3p</i>	<i>B11avgbr.3p</i>	<i>b11mnbr.3p</i>
EQ6 Input File Name	<i>B11Mxbr.6i</i> <i>11Mxbr1.6i</i> <i>11Mxbr4.6i</i>	<i>B11Avgbr.6i</i> <i>11Avgbr1.6i</i> <i>11Avgbr4.6i</i>	<i>B11Mnbr.6i</i> <i>11Mnbr1.6i</i> <i>11Mnbr4.6i</i>
EQ6 Output File Name	<i>b11mxbr.6o</i> <i>11mxbr1.6o</i> <i>11mxbr4.6o</i>	<i>B11avgbr.6o</i> <i>11avgbr1.6o</i> <i>11avgbr4.6o</i>	<i>b11mnbr.6o</i> <i>11mnbr1.6o</i> <i>11mnbr4.6o</i>
Lookup Table File Name	<i>bin11mxbrLT.xls</i>	<i>Bin11avgbrLT.xls</i>	<i>bin11mnbrLT.xls</i>

Source: Output DTN: MO0310SPAPCEUA.002.

6.12.4.2.3 Results of Bromide in Seepage Waters

Figure 6.12-1 depicts the total Br concentration as the seepage water is evaporated: when added to the starting waters in concentrations found in the porewaters it is used as inputs to the THC seepage model. Concentrations of Br can become large as evaporation progresses and brines become more and more concentrated. Below a relative humidity of approximately 70 percent, the results start to show the temperature dependency of KBr saturation; higher Br concentrations tend to be possible at lower temperatures. At very low relative humidity, the Br concentrations in solution can become rather high, on the order of 1 to 3 molal. These concentrations are similar to those found in the dust leachate samples (Section 6.12.4.2.4). At the lowest lookup table RH of 65 percent, the maximum Br concentration is 0.4 molal, and is typically much lower.

Also shown in this section are the effects of Br addition on predicted pH and ionic strength (Figures 6.12-2 and 6.12-3). Over the entire RH range examined, the presence of Br in solution causes no noticeable change in the predicted pH values. The effect on ionic strength is small but increases with evaporation. It is greatest at low relative humidity, where the uncertainty can be as large as 1 to 5 molal. At 65 percent RH, only the 40°C data show a significant deviation—in the high Br case, the predicted ionic strength is lowered by ~1 molal (~8 percent relative).

Source: Output DTN: MO0310SPAPCEUA.002.

Figure 6.12-1. Uncertainty in Bin 11 Br Concentrations Using the Br Values from Porewater

Source: Output DTN: MO0310SPAPCEUA.002.

Figure 6.12-2. Uncertainty in Bin 11 Ionic Strength Due to Adding Br

Source: Output DTN: MO0310SPAPCEUA.002.

Figure 6.12-3. Uncertainty in Bin 11 pH Due to Adding Br

Figure 6.12-4 shows the effect on molar ratios that are of importance to waste package corrosion. The ratios only deviate significantly at lower relative humidity, where there would be an increase in halide concentration with respect to NO_3^- and SO_4^{2-} , and these are below the lowest RH values reported in the TSPA-LA lookup table and, therefore, of negligible impact.

Source: Output DTN: MO0310SPAPCEUA.002.

Figure 6.12-4. Uncertainty in Bin 11 Molar Ratios Due to Adding Br

6.12.4.2.4 Results of Bromide in Dust Leachate

The presence of Br in the dust leachate waters may be due to the addition of amounts of LiBr as a tracer in construction water (Peterman et al. 2003 [DIRS 162819]), reported as containing a median 0.34 Cl/Br ratio (Davis et al. 1998 [DIRS 162782], Table 6). In waters above the halite divide, halides (Br and Cl) are present in the natural environment in consistent ratios ($\text{Cl}/\text{Br} \sim 3.3 \times 10^2$) (Krauskopf 1979 [DIRS 105909], Table 12-4; White et al. 1963 [DIRS 163752], p. F13, Tables 13 to 18; and Table 6.12-20). Ten measurements of this halide ratio in Topopah Spring welded tuff unit gave a median value of 518 (Davis et al. 1998 [DIRS 162782], Table 6). Chlorine-bromine ratios in the dust leachate waters are much lower than this (Table 6.12-24), and are as much as 10-fold lower than the seepage water ratios from Table 6.12-21, suggesting that as much as 90 percent of the Br in the dust is from construction water. Whether the Br source is the construction water or is from seepage water interacting with dusts in the ESF, it can be said, by analogy with the calculation results shown on Figure 6.12-1 for seepage water, that the concentration of Br in the dust leachate brines will increase as a result of evaporation, even after the solution reaches saturation with respect to halite. The evaporative concentration of Br beyond the halite divide is confirmed by Hem (1985 [DIRS 115670], p. 146).

Comparing Figure 6.12-1 with Figure 6.12-5 shows the evaporative concentration of Br for the porewaters in the mountain is consistent with this same 10-fold increase in the dust leachate results. This suggests that the concentrations of chloride and other species of interest are reasonably accurate even though there could be some impact from construction waters. There is some uncertainty in the *Data0.yppf* database with respect to Br species, especially Ca and Mg bromide solids (BSC 2004 [DIRS 169863]). However, these chemical species are extremely soluble and do not affect the results shown in Figure 6.12-5 in a significant way. Therefore, this section reports the actual values calculated in Section 6.10.

Source: Output DTN: MO0310SPAPCELA.002.

Figure 6.12-5. Comparative Evaporative Concentration of Br in Dust Leachate Water Lookup Tables

Table 6.12-24. Cl:Br ratios of Dust Leachate Samples

Data From Table 4.1-19				
Lab No.	Field No.	Cl (ppm)	Br (ppm)	Cl:Br
C-186077	SPC00573607	260	14	18.57
C-186080	SPC00573610	162	34	4.76
C-186081	SPC00573611	200	56	3.57
C-186082	SPC00573612	154	50	3.08
C-186084	SPC00573614	130	24	5.42
C-186085	SPC00573615	162	22	7.36
C-186086	SPC00573616	130	26	5.00
C-186087	SPC00573617	140	20	7.00
C-186088	SPC00573618	114	16	7.13
C-186089	SPC00573619	200	22	9.09
C-186090	SPC00573620	56	6	9.33
C-186091	SPC00573622	182	10	18.20
C-186092	SPC00573623	180	22	8.18
C-186093	SPC00573624	240	54	4.44
C-186094	SPC00573625	300	26	11.54
C-186095	SPC00573626	200	26	7.69
C-186096	SPC00573627	260	34	7.65
C-186097	SPC00573628	160	18	8.89
C-186098	SPC00573629	184	38	4.84
C-186099	SPC00573630	196	28	7.00
C-186100	SPC00573631	220	64	3.44
C-186101	SPC00573632	220	28	7.86
C-186102	SPC00573633	114	22	5.18
Data From Table 4.1-20				
Lab. No./ Sample No.	Mesh Size			
C-203116/ 00574980B	200 to 325	98	4	24.50
C-203117/ 00574980C	<325	154	8	19.25
C-203118/ 00574981A	60 to 200	74	4	18.50
C-203119/ 00574981B	200 to 325	280	44	6.36
C-203120/ 00574981C	<325	320	6	53.33
C-203121/ 00574982A	60 to 200	86	4	21.50
C-203122/ 00574982B	200 to 325	118	6	19.67
C-203123/ 00574982C	<325	170	12	14.17
C-203124/ 00574983A	60 to 200	114	8	14.25
C-203125/ 00574983B	200 to 325	260	10	26.00
C-203126/ 00574983C	<325	360	10	36.00
C-203127/ 00574984A	60 to 200	128	10	12.80
C-203128/ 00574984B	200 to 325	-	-	-

Table 6.12-24. Cl:Br ratios of Dust Leachate Samples (Continued)

Data From Table 4.1-20				
Lab No.	Field No.	Cl (ppm)	Br (ppm)	Cl:Br
C-203129/ 00574984C	<325	220	18	12.22
C-203130/ 00574985A	60 to 200	170	20	8.50
C-203131/ 00574985B	200 to 325	168	14	12.00
C-203132/ 00574985C	<325	166	16	10.38
C-203133/ 00574986A	60 to 200	96	6	16.00
C-203134/ 00574986B	200 to 325	170	10	17.00
C-203135/ 00574986C	<325	220	14	15.71
C-203136/ 00574987A	60 to 200	188	2	94.00
C-203137/ 00574987B	200 to 325	360	42	8.57
C-203138/ 00574987C	<325	320	32	10.00
C-203139/ 00574990A	60 to 200	88	10	8.80
C-203140/ 00574990B	200 to 325	102	16	6.38
C-203141/ 00574990C	<325	136	22	6.18
C-203142/ 00574991A	60 to 200	88	12	7.33
C-203143/ 00574991B	200 to 325	76	10	7.60
C-203144/ 00574991C	<325	82	12	6.83
C-203145/ 00574992A	60 to 200	98	6	16.33
C-203146/ 00574992B	200 to 325	82	<1.6	-
C-203147/ 00574992C	<325	166	2	83.00
Average				14.88
Min.				3.08
Max.				94.00

Source: Output DTN: MO0310SPAPCEUA.002.

All 52 of the calculated EQ6 output files listed on Table 6.10-12 were extracted using GETEQDATA software thus creating *newDustMOALT.xls* (archived in DTN: MO0310SPAPCELA.002). This file was then used to create Figure 6.12-5, which shows the evaporative concentration of Br as a function of relative humidity. For many of the 52 waters, Br can concentrate to values above 1 molal reaching up to ~8 molal in some cases. The 9 to 12 waters exceeding 5 molal Br are taken from dust leachate Bins 2, 3, 4 and 6, calculated at 40°C. Examination of the results in *newDustMOALT.xls* indicates that the higher Br concentrations are associated with the lower temperature calculation runs, and are not likely to occur because at low temperatures the relative humidity in the drifts should be high, and concentrated brines would not be stable.

In order to account for potential Br contamination due to construction water, Br concentrations in the dust leachates were reduced by a factor of 10 and a sensitivity calculation run was made to investigate the impacts of this reduction. The factor of ten reduction was determined by comparing the average statistics on the Cl:Br ratio for the dust leachate (14.88) calculated from the data in Tables 4.1-19 and 4.1-20 as shown on Table 6.12-24 with the average Cl:Br ratio for the seepage water (267) shown in Table 6.12-21.

Table 6.12-25 lists the base-case file and the file names for the adjusted EQ3/6 calculations. The adjusted EQ3 3i file Br concentration is reduced by a factor of 10 and the EQ6 evaporation calculation is rerun using the appended EQ3 pickup file.

Table 6.12-25. Br Dust Leachate Uncertainty Analysis EQ3/6 Input and Output Files

Base-Case File	Adjusted Input and Output Files	GetEQData Output Spreadsheet File
<i>d1c3i07.6o</i> (Table 6.10-14)	<i>Bin1_Br.3i</i> , <i>Bin1_Br.3p</i> , <i>Bin1_Br.3o</i> , <i>Bin1_Br.6i</i> , <i>Bin1_Br.6o</i>	<i>Dust Br sensitivity study Bin 1.xls</i>

Source: Output DTN: MO0310SPAPCEUA.002.

Figures 6.12-6 through 6.12-10 show the results of the sensitivity study. The results indicate that there is no significant difference in pH, ionic strength, Cl or N concentration above an activity of water of approximately 0.47. However, some differences in these values are evident below a water activity of 0.47. Still, the endpoint composition of the two calculations is essentially the same. This suggests that including the effects of Br from traced construction water does not significantly impact the results of the chemistry provided in the lookup tables.

Source: Output DTN: MO0310SPAPCEUA.002.

Figure 6.12-6. Change in Predicted pH Due to Adjustment of Dust Leachate Bin 1 Br Concentration

Source: Output DTN: MO0310SPAPCEUA.002.

Figure 6.12-7. Change in Predicted Ionic Strength Due to Adjustment of Dust Leachate Bin 1 Br Concentration

Source: Output DTN: MO0310SPAPCEUA.002.

Figure 6.12-8. Change in Predicted N Concentrations Due to Adjustment of Dust Leachate Bin 1 Br Concentration

Source: Output DTN: MO0310SPAPCEUA.002.

Figure 6.12-9. Change in Predicted Br Concentrations Due to Adjustment of Dust Leachate Bin 1 Br Concentration

Source: Output DTN: MO0310SPAPCEUA.002.

Figure 6.12-10. Change in Predicted Cl Concentrations Due to Adjustment of Dust Leachate Bin 1 Br Concentration

6.12.4.3 Extrapolating $p\text{CO}_2$ Values Beyond Lookup Tables

As discussed in Section 6.13.3, extrapolation can be made when $p\text{CO}_2$ is outside the given range of the EBS seepage and dust leachate lookup tables. This sensitivity study gives the predictive range to which the lookup tables can be extrapolated. Results indicate that valid linear extrapolation as a function of $p\text{CO}_2$ can be performed for values of ionic strength, and chloride and nitrogen (mostly nitrate) concentrations, and log scale extrapolations for pH.

6.12.4.3.1 Calculation Framework

Two calculation cases are run for each of the base-case files (Table 6.12-15) to bound the effects of the possible range of $p\text{CO}_2$. Based on the total possible range of in-drift $p\text{CO}_2$ (1.75×10^{-2} to 2.29×10^{-5} atmospheres) discussed in Section 6.7.2.2, there is a possibility that the lookup tables used in the TSPA-LA model could be outside the 10^{-2} to 10^{-4} bar range specified for the creation of the seepage lookup tables (Section 6.9). A sensitivity calculation run is made using $p\text{CO}_2 = 10^{-5}$ bar and a sensitivity run using $p\text{CO}_2 = 10^{-1}$ bar. These input and output files are listed on Tables 6.12-26 and 6.12-27 for the seepage water and dust leachate water, respectively.

Table 6.12-26. Input and Output Files for Seepage Bin 11 Analysis of $p\text{CO}_2$

$p\text{CO}_2$	Input Files	Output Files
10^{-1} bar	11c1t7e.6i	11c1t7e.6o
10^{-5} bar	11c5t7e.6i	11c5t7e.6o

Source: Output DTN: MO0310SPAPCEUA.002.

Table 6.12-27. Input and Output Files for Dust Leachate Bin 5 Analysis of $p\text{CO}_2$

$p\text{CO}_2$	Input Files	Output Files
10^{-1} bar	d5c1t07.6i	d5c1t07.6o
10^{-5} bar	d5c5t07.6i	d5c5t07.6o

Source: Output DTN: MO0310SPAPCEUA.002.

6.12.4.3.2 Seepage Water Results

GETEQDATA software has been used to extract the appropriate output from the output files. The resulting *Seepage CO₂ uncert.xls* is used to create Figures 6.12-11 through 6.12-14. This spreadsheet is archived in DTN: MO0310SPAPCEUA.002.

Figure 6.12-11 shows the variation in pH when $p\text{CO}_2$ gas values fall outside the normal range of the provided lookup tables. The trend is about half a pH unit increase for every order of magnitude decrease in $p\text{CO}_2$ below 10^{-4} bar, and nearly one pH unit decrease when increasing $p\text{CO}_2$ above 10^{-2} bar. High-pressure $p\text{CO}_2$ extrapolation of pH could result in an additional error of nearly half a pH unit, but only at this extreme $p\text{CO}_2$ of 10^{-1} bar. This error would at most scale log linearly with $p\text{CO}_2$ and, therefore, at $p\text{CO}_2 = 2 \cdot 10^{-2}$ bar (high end of in-drift range); this error can be at most 0.15 pH and is, thus, small compared to total uncertainty.

For ionic strength and N, there is only a small dependence upon $p\text{CO}_2$ and only at low RH (Figures 6.12-12 and 6.12-14). Cl however, shows some linearly predictable trends. The values at 10^{-1} bar show more variation, as the predictable trends are not as uniform (Figure 6.12-13). These trends are strongly associated with the activity at which calcite and halite precipitate.

Source: Output DTN: MO0310SPAPCEUA.002.

Figure 6.12-11. Variation in Bin 11 Base-Case pH as a Function of $p\text{CO}_2$

Source: Output DTN: MO0310SPAPCEUA.002.

Figure 6.12-12. Variation in Bin 11 Base-Case Ionic Strength as a Function of pCO_2

Source: Output DTN: MO0310SPAPCEUA.002.

Figure 6.12-13. Variation in Bin 11 Base-Case Total Elemental Cl as a Function of pCO_2

Source: Output DTN: MO0310SPAPCEUA.002.

Figure 6.12-14. Variation in Bin 11 Base-Case Total Elemental N as a Function of $p\text{CO}_2$

6.12.4.3.3 Dust Leachate Water Results

GETEQDATA software is used to extract the appropriate output from the output files. The resulting *Dust CO₂ uncert.xls* is used to create the following figures (Figures 6.12-15 through 6.12-18). This spreadsheet is archived in DTN: MO0310SPAPCEUA.002.

Figure 6.12-15 shows the range of uncertainty that needs to be applied to the pH results when $p\text{CO}_2$ gas values fall outside the normal range of the provided lookup tables. This range is about half a pH unit when decreasing $p\text{CO}_2$ below 10^{-4} bar, and about half a pH unit when increasing $p\text{CO}_2$ above 10^{-2} bar. Results within this large range of $p\text{CO}_2$ are very regular and any interpolation errors are expected to be negligible.

For the other three lookup table parameters, there are negligible dependencies upon the $p\text{CO}_2$. Figures 6.12-16 through 6.12-18 show ionic strength, chloride, and nitrogen molalities, respectively, are insensitive to $p\text{CO}_2$. These parameters therefore add no measurable uncertainty or error to any extrapolations based upon $p\text{CO}_2$.

Source: Output DTN: MO0310SPAPCEUA.002.

Figure 6.12-15. Variation in Bin 5 Base-Case pH as a Function of pCO_2

Source: Output DTN: MO0310SPAPCEUA.002.

Figure 6.12-16. Variation in Bin 5 Base-Case Ionic Strength as a Function of pCO_2

Source: Output DTN: MO0310SPAPCEUA.002.

Figure 6.12-17. Variation in Bin 5 Base-Case Total Elemental Cl as a Function of $p\text{CO}_2$

Source: Output DTN: MO0310SPAPCEUA.002.

Figure 6.12-18. Variation in Bin 5 Base-Case Total Elemental N as a Function of $p\text{CO}_2$

6.12.4.4 MineralSuppressions

Three minerals, cryolite, glaserite and magnesite, have been identified as candidates for sensitivity studies to document the impact of mineral suppressions on our analyses (Table 6.5-2). This is based on their inclusion or exclusion in the thermodynamic modeling approach that is used, as discussed in Section 6.5.

Table 6.12-28 documents the base-case input files and associated output files used to investigate the suppression or inclusion of these minerals. The base-case input file is modified by either including or removing the mineral in the "Alter/Suppress Options" input block of the EQ6 *.6i data file. The results are extracted into a Microsoft Excel spreadsheet using the GETEQDATA software. This spreadsheet (*Mineral suppressions.xls* archived in DTN: MO0310SPAPCEUA.002) is used to create the figures and determine the results shown in the following subsections.

Table 6.12-28. Traceability Roadmap for Mineral Suppression EQ6 Sensitivity Cases

Suppression Case	Base-Case Input File	Altered Input File	Output file
Cryolite	11c2t4e.6i (Table 6.9-5)	11crysupsup.6i	11crysupsup.6o
Glaserite	11c3t7e.6i (Table 6.12-9)	11glas.6i	11glas.6o
Magnesite	11c3t7e.6i (Table 6.12-9)	11mag.6i	11mag.6o

Source: Output DTN: MO0310SPAPCEUA.002.

6.12.4.4.1 Cryolite

In the modeling work performed to establish the mineral suppression tables (Tables 6.5-2 and 6.6-2), cryolite did not precipitate; therefore, it was not suppressed when creating the seepage lookup tables (Sections 6.5, 6.6, and 6.9), yet it precipitated in a few cases (Table 6.13-6). Cryolite (Na_3AlF_6) is a halide mineral that is associated with pegmatite veins in granite and gneiss (Palache et al. 1951 [DIRS 162280], p. 113); it commonly forms at higher temperature and pressure conditions not relevant to the repository and would have normally been suppressed on this basis. However, during the literature review that was performed, cryolite was also found to precipitate in fluid inclusions where the end member solutions are Na-K-Ca-Cl- HCO_3 brines. The minerals associated with cryolite in these fluid inclusions are nahcolite, halite, sylvite and fluorite (Buhn and Rankin 1999 [DIRS 163753]). These minerals are commonly found in evaporite deposits and are present in many of the lookup table results as precipitates. The naturally occurring association with common evaporite minerals would justify the inclusion of cryolite as a potential precipitate in our system. Therefore, this sensitivity analysis was conducted to determine the potential impact to the lookup tables.

Total aqueous concentrations for Na, Al, and F are shown on Figure 6.12-19. Also plotted are pH and the moles of cryolite precipitated in the base-case results. Figure 6.12-19 also shows that with the exception of the Al concentrations, there is no major impact to the base-case files from the precipitation of cryolite. The Al concentrations are affected by approximately two orders of magnitude, but because Al concentrations are less than 10^{-10} molal, the pH and other parameters of interest are unaffected.

Source: Output DTN: MO0310SPAPCEUA.002.

Figure 6.12-19. Comparison of Base-Case EQ6 Results with those of the Cryolite-Suppressed Modeling Run

6.12.4.4.2 Glaserite

As reported in Table 6.5-2, glaserite ($NaK_3(SO_4)_2$) is suppressed due to the uncertain nature of the values reported in the *Data0.ypf* thermodynamic database. This sensitivity calculation run documents the potential changes that could occur if glaserite is allowed to precipitate in the analyses. The *Data0.ypf* database includes two sets of data; the set that was used is the single 25°C log K value of -3.8027. Therefore, the modeling calculation runs done at 70°C are not fully representative, but do indicate the potential changes to the output results that could occur with inclusion.

Figure 6.12-20 shows the comparative results of the base case with the inclusion of glaserite for pH, S, Na, and K. The largest change is the difference in endpoint water activity. With the glaserite present, the endpoint of the calculated model run is lowered by about 15 percent. The pH change is less than half a unit when the base-case calculation run ends. The aqueous solute concentrations do not vary much (less than 1 order of magnitude). The pH shift at the lowest water activity used in the lookup tables ($a_w = 0.65$) is just under 0.2 pH units.

Source: Output DTN: MO0310SPAPCEUA.002.

Figure 6.12-20. Comparison of Base-Case Results to those of the Same Modeling Run with Glaserite Unsuppressed

6.12.4.4.3 Magnesite

As reported on Table 6.5-2, according to Eugster and Hardie (1978 [DIRS 100743]) magnesite can be associated with salt deposits. However, it is uncertain whether it is associated with the diagenesis of salt deposits at temperatures and pressures higher than 100°C and 1 atmosphere respectively, or with lower temperatures and pressures such as those anticipated in the repository. The sensitivity analysis is conducted to evaluate the possible effects to our model results. The results indicate that even with the inclusion of magnesite in the modeling calculation run, it does not precipitate in the base-case file. Therefore, with this limited sensitivity study, it is concluded that there is no impact to the results.

6.12.4.5 Mineral Precipitation

Supplemental to the information found on Tables 6.5-2 and 6.5-3, Table 6.12-28a includes natural analog information and the mineral inclusion (or suppression) criteria as discussed in Section 6.5.5. As indicated, all the minerals listed on Tables 6.5-3 and 6.12-28a have analog information that allow for their precipitation in this model, the information here corroborates the minerals that are precipitating in this model.

Cryolite (Table 6.10-1), which was included in the seepage modeling runs, but suppressed in the dust leachate runs, has analog information that suggests mineral suppression indicated in EQ3/6

calculations would be warranted. It may be possible for cryolite to precipitate under repository conditions.

Section 6.12.4.4.1 documents an uncertainty calculation that indicates a suppression of cryolite has virtually no impact on the seepage lookup table results except for the aluminum output (Figure 6.12-19). This portion of the output can be affected by two orders of magnitude as the water activity decreases. Cryolite formation is predicted in some of the lookup tables representing bins 9, 10, and 11. As shown in Figure 6.12-19, the impact is not significant since the aluminum concentrations are less than 10^{-10} mol/kg H_2O , thereby having no effect on the bulk chemistry.

Table 6.12-28a. Natural Analog Information for the Inclusion of Minerals Not Reported in Section 6.5

Mineral Name (if available)	Formula	Criteria Selected ^a	Rationale	References
Calcium nitrate	$Ca(NO_3)_2$	Criterion 3	Less hydrated phase of nitrocalcite	See below
	$Ca(NO_3)_2 \cdot 3H_2O$	Criterion 3	Less hydrated phase of nitrocalcite	See below
Nitrocalcite	$Ca(NO_3)_2 \cdot 4H_2O$	Criterion 3	Water soluble salt associated with niter deposits in caves and lake beds	Palache et al. 1951 [DIRS 162280], pp. 306 to 307
Erionite	$K_{1.5}Na_{0.9}Ca_{0.9}Al_{4.2}Si_{13.8}O_{36} \cdot 13H_2O$	Criterion 3	Zeolite mineral known to form in sedimentary saline, non-marine environments	Frye 1981 [DIRS 161804], p. 524 Hay 1966 [DIRS 105965], Table 4
Nahcolite	$NaHCO_3$	Criterion 3	Associated with trona and other playa or salt bed minerals	Palache et al. 1951 [DIRS 162280], p. 135
Pirssonite	$Na_2Ca(CO_3)_2 \cdot 2H_2O$	Criterion 3	Associated with trona and thenardite and is found in clays in dry lake beds	Palache et al. 1951 [DIRS 162280], p. 233
Potassium bromide	KBr	Criterion 3	Deliquescent mineral that maintains a saturated solution at 84% RH at 20°C and 69% RH at 100°C	Weast 1984 [DIRS 106170], p. E-42
Kalinite	$KHCO_3$	Criterion 3	Associated with trona	Palache et al. 1951 [DIRS 162280], p. 136
Brucite	$Mg(OH)_2$	Criterion 3	Associated with contact metamorphosed limestone in association with calcite, dolomite and magnesite. This would be analogous to calcite alteration on the surface of the hot waste packages. In the modeling runs brucite only forms in one dust leachate lookup table at 100°C Brucite is also found in crystalline limestone; the chief component of which is calcite	Frye 1981 [DIRS 161804], p. 568 Klein and Hurlbut 1977 [DIRS 105907], p. 316

Table 6.12-28a. Natural Analog Information for the Inclusion of Minerals Not Reported in Section 6.5 (Continued)

Mineral Name (if available)	Formula	Criteria Selected ^a	Rationale	References
Darapskite	Na ₃ (NO ₃)(SO ₄): H ₂ O	Criterion 3	Associated soda-niter, niter, halite, and anhydrite. Also occurs in nitrate and sulfate deposits	Palache et al. 1951 [DIRS 162280], p. 310
Thermonatrite	Na ₂ CO ₃ :H ₂ O	Criterion 3	Associated with trona and is found as an efflorescence on soil in arid regions and as a deposit from saline lakes	Palache et al. 1951 [DIRS 162280], p. 224
Villiaumite	NaF	Criterion 3	Deliquescent mineral that maintains a saturated solution at 96% RH at 100°C	Weast 1984 [DIRS 106170], p. E-42

NOTE: ^a Criterion described in Section 6.5.4.1; briefly, Criterion 3 means analytical or analogue information is available to support inclusion or exclusion of mineral.

6.12.5 Implementing Uncertainties in the TSPA-LA Abstraction Lookup Tables

EBS chemical environments abstractions are documented for use by the TSPA-LA in the form of lookup tables identified in Sections 6.7, 6.9, 6.10, 6.15.1.1, and 6.15.1.2. Seepage evaporation and dilution lookup tables and dust deliquescence lookup tables are archived in the following DTNs:

- MO0304SPACSALT.000
- MO0310SPADLALT.001
- MO0310SPADLHTL.000.

The subsequent sections provide the details on the determination and guidelines on the treatment of uncertainties by the TSPA-LA.

6.12.5.1 Uncertainties that Are Negligible and Not Included

Degradation of stainless steel in ground support components, treatment of bromide in the abstraction, extrapolation of $p\text{CO}_2$ values outside the range of the lookup tables, and alternate mineral suppressions are all shown to have a negligible effect on the uncertainties in EBS chemical environments abstractions. Evidence for the relative insignificance of those processes is presented in previous Section 6.12.4.

6.12.5.2 Uncertainty Distributions for TSPA-LA Lookup Tables

As shown in Tables 6.12-1, 6.12-4, and 6.12-8, uncertainty in the model output stems from two sources, IDPS model uncertainty and the uncertainty due to binning (or lookup table) variability. These two types of uncertainty have to be accounted for in the TSPA-LA. The IDPS model uncertainties in chemical parameters relevant to the TSPA-LA, and in deliquescence RH, are summarized in Table 6.12-1. Binning uncertainties for seepage and dust can be found in Tables 6.12-4 and 6.12-8, respectively.

The lookup table results in Section 6.13 (Figures 6.13-29 and 6.13-38) indicate that, in all cases, once the halite divide is crossed, the $\text{Cl}:\text{NO}_3$ ratio can only decrease. These results indicate that, at relative humidity below the halite divide, a limit can be placed on the uncertainty of this value. In most lookup table cases, there is another divide (sylvite) that further ensures this limit. Tables 6.12-29 and 6.12-30 are a compilation of the $\text{Cl}:\text{NO}_3$ ratio at the halite divide for all simulations. These tables were created by extracting the relevant information from the lookup table DTNs: MO0304SPACSALT.000, MO0310SPADLALT.001, and MO0310SPADLHTL.000, and calculating the ratios.

6.12.5.3 Specific Guidance for TSPA-LA Implementation

The lookup tables summarizing seepage waters and dust deliquescence chemistries must be implemented in the TSPA-LA with the associated uncertainties. Carbon dioxide partial pressure lookup tables, as taken from the THC model results, are shown in Tables 6.7-1 through 6.7-5 and are archived in DTN: MO0308SPACO2GL.001. Seepage lookup tables and low- and high-temperature dust lookup tables are archived in DTNs: MO0304SPACSALT.000 (DTN: MO0310SPAPCEGS.000 for the TSPA-LA model use), MO0310SPADLALT.001, and MO0310SPADLHTL.000, respectively.

Quantification of the uncertainties in parameters that will feed the TSPA-LA is developed above and includes the following parameters:

- Ionic strength
- Chloride concentration
- Chloride to nitrate ratio
- pH
- Deliquescence RH point.

Nitrate uncertainty is calculated using the chloride and chloride-to-nitrate ratio uncertainties to account for any correlation as discussed in the following paragraphs.

Because distinct water compositions are provided in the lookup tables along an evolutionary evaporative path using the IDPS model, any uncertainty distribution selected at the beginning of the evaporative path can be maintained throughout any given TSPA-LA model realization.

Table 6.12-29. Cl:NO₃ Molal Ratio for Seepage at the Halite Chemical Divide

Bin Number	Temp (°C)	pCO ₂ (bar)	Halite Divide Cl:NO ₃ Molal Ratio	Halite Divide Log Cl:NO ₃ Molal Ratio
1	70	0.0001	15.46	1.19
	40	0.0001	15.46	1.19
	100	0.0001	15.46	1.19
	70	0.001	15.46	1.19
	40	0.001	15.46	1.19
	100	0.001	15.46	1.19
	70	0.01	15.46	1.19
	40	0.01	15.46	1.19
	100	0.01	15.46	1.19
2	70	0.0001	9.19	0.96
	40	0.0001	9.19	0.96
	100	0.0001	9.19	0.96
	70	0.001	9.19	0.96
	40	0.001	9.19	0.96
	100	0.001	9.19	0.96
	70	0.01	9.19	0.96
	40	0.01	9.19	0.96
	100	0.01	9.19	0.96
3	70	0.0001	18.30	1.26
	40	0.0001	18.30	1.26
	100	0.0001	18.30	1.26
	70	0.001	18.30	1.26
	40	0.001	18.30	1.26
	100	0.001	18.30	1.26
	70	0.01	18.30	1.26
	40	0.01	18.30	1.26
	100	0.01	18.30	1.26
4	70	0.0001	7.74	0.89
	40	0.0001	7.74	0.89
	100	0.0001	7.74	0.89
	70	0.001	7.74	0.89
	40	0.001	7.74	0.89
	100	0.001	7.74	0.89
	70	0.01	7.74	0.89
	40	0.01	7.74	0.89
	100	0.01	7.74	0.89

Table 6.12-29. Cl:NO₃ Molal Ratio for Seepage at the Halite Chemical Divide (Continued)

Bin Number	Temp (°C)	pCO ₂ (bar)	Halite Divide Cl:NO ₃ Molal Ratio	Halite Divide Log Cl:NO ₃ Molal Ratio
5	70	0.0001	14.77	1.17
	40	0.0001	14.77	1.17
	100	0.0001	14.77	1.17
	70	0.001	14.77	1.17
	40	0.001	14.77	1.17
	100	0.001	14.77	1.17
	70	0.01	14.77	1.17
	40	0.01	14.77	1.17
	100	0.01	14.77	1.17
6	70	0.0001	31.91	1.50
	40	0.0001	31.91	1.50
	100	0.0001	31.91	1.50
	70	0.001	31.91	1.50
	40	0.001	31.91	1.50
	100	0.001	31.91	1.50
	70	0.01	31.91	1.50
	40	0.01	31.91	1.50
	100	0.01	31.91	1.50
7	70	0.0001	31.70	1.50
	40	0.0001	31.70	1.50
	100	0.0001	31.70	1.50
	70	0.001	31.70	1.50
	40	0.001	31.70	1.50
	100	0.001	31.70	1.50
	70	0.01	31.70	1.50
	40	0.01	31.70	1.50
	100	0.01	31.70	1.50
8	70	0.0001	14.12	1.15
	40	0.0001	14.12	1.15
	100	0.0001	14.12	1.15
	70	0.001	14.12	1.15
	40	0.001	14.12	1.15
	100	0.001	14.12	1.15
	70	0.01	14.12	1.15
	40	0.01	14.12	1.15
	100	0.01	14.12	1.15

Table 6.12-29. Cl:NO₃ Molal Ratio for Seepage at the Halite Chemical Divide (Continued)

Bin Number	Temp (°C)	pCO ₂ (bar)	Halite Divide Cl:NO ₃ Molal Ratio	Halite Divide Log Cl:NO ₃ Molal Ratio
9	70	0.0001	2.37	0.37
	40	0.0001	2.37	0.37
	100	0.0001	2.37	0.37
	70	0.001	2.37	0.37
	40	0.001	2.37	0.37
	100	0.001	2.37	0.37
	70	0.01	2.37	0.37
	40	0.01	2.37	0.37
	100	0.01	2.37	0.37
10	70	0.0001	14.11	1.15
	40	0.0001	14.11	1.15
	100	0.0001	14.11	1.15
	70	0.001	14.11	1.15
	40	0.001	14.11	1.15
	100	0.001	14.11	1.15
	70	0.01	14.11	1.15
	40	0.01	14.11	1.15
	100	0.01	14.11	1.15
11	70	0.0001	10.31	1.01
	40	0.0001	10.31	1.01
	100	0.0001	10.31	1.01
	70	0.001	10.31	1.01
	40	0.001	10.31	1.01
	100	0.001	10.31	1.01
	70	0.01	10.31	1.01
	40	0.01	10.31	1.01
	100	0.01	10.31	1.01

Source: Output DTN: MO0311SPAEP MUT.000, *halite divide ratio for seepage.xls*.

Table 6.12-30. Cl:NO₃ Molal Ratio for Dust at the Halite Chemical Divide

Bin Number	Temperature (°C)	pCO ₂ (bar)	Halite Divide Cl:NO ₃ Molal Ratio	Halite Divide Log Cl:NO ₃ Molal Ratio
1	40	0.01	0.47	-0.33
	40	0.001	0.47	-0.32
	40	0.0001	0.47	-0.32
	70	0.01	0.42	-0.38
	70	0.001	0.42	-0.38
	70	0.0001	0.42	-0.38
	100	0.01	0.42	-0.38
	100	0.001	0.42	-0.38
	100	0.0001	0.42	-0.38
	120	0.01	0.42	-0.38
	120	0.001	0.42	-0.38
	120	0.0001	0.42	-0.38
	140	0.0001	0.42	-0.38
	140	0.001	0.42	-0.38
	140	0.01	0.42	-0.38
2	40	0.01	0.81	-0.09
	40	0.001	0.81	-0.09
	40	0.0001	0.81	-0.09
	70	0.01	0.81	-0.09
	70	0.001	0.81	-0.09
	70	0.0001	0.81	-0.09
	100	0.01	0.81	-0.09
	100	0.001	0.81	-0.09
	100	0.0001	0.81	-0.09
	120	0.01	0.81	-0.09
	120	0.001	0.81	-0.09
	120	0.0001	0.81	-0.09
	140	0.0001	0.81	-0.09
	140	0.001	0.80	-0.09
	140	0.01	0.81	-0.09

Table 6.12-30. Cl:NO₃ Molal Ratio for Dust at the Halite Chemical Divide
(Continued)

Bin Number	Temperature (°C)	pCO ₂ (bar)	Halite Divide Cl:NO ₃ Molal Ratio	Halite Divide Log Cl:NO ₃ Molal Ratio
3	40	0.01	1.14	0.06
	40	0.001	1.15	0.06
	40	0.0001	1.06	0.03
	70	0.01	1.15	0.06
	70	0.001	1.15	0.06
	70	0.0001	1.15	0.06
	100	0.01	1.15	0.06
	100	0.001	1.15	0.06
	100	0.0001	1.15	0.06
	120	0.01	1.15	0.06
	120	0.001	1.15	0.06
	120	0.0001	1.15	0.06
	140	0.0001	1.01	0.00
	140	0.001	1.00	0.00
	140	0.01	1.15	0.06
4	40	0.01	0.77	-0.11
	40	0.001	0.77	-0.11
	40	0.0001	0.77	-0.11
	70	0.01	0.77	-0.11
	70	0.001	0.77	-0.11
	70	0.0001	0.77	-0.11
	100	0.01	0.77	-0.11
	100	0.001	0.77	-0.11
	100	0.0001	0.77	-0.11
	120	0.01	0.77	-0.11
	120	0.001	0.77	-0.11
	120	0.0001	0.77	-0.11
	140	0.0001	0.77	-0.11
	140	0.001	0.77	-0.11
	140	0.01	0.77	-0.11

Table 6.12-30. Cl:NO₃ Molal Ratio for Dust at the Halite Chemical Divide (Continued)

Bin Number	Temperature (°C)	pCO ₂ (bar)	Halite Divide Cl:NO ₃ Molal Ratio	Halite Divide Log Cl:NO ₃ Molal Ratio
5	40	0.01	0.87	-0.06
	40	0.001	0.87	-0.06
	40	0.0001	0.87	-0.06
	70	0.01	0.87	-0.06
	70	0.001	0.87	-0.06
	70	0.0001	0.87	-0.06
	100	0.01	0.87	-0.06
	100	0.001	0.87	-0.06
	100	0.0001	0.87	-0.06
	120	0.01	0.87	-0.06
	120	0.001	0.87	-0.06
	120	0.0001	0.87	-0.06
	140	0.0001	0.87	-0.06
	140	0.001	0.87	-0.06
	140	0.01	0.87	-0.06
6	40	0.01	2.18	0.34
	40	0.001	2.34	0.37
	40	0.0001	2.39	0.38
	70	0.01	2.45	0.39
	70	0.001	2.45	0.39
	70	0.0001	2.45	0.39
	100	0.01	2.45	0.39
	100	0.001	2.45	0.39
	100	0.0001	2.45	0.39
	120	0.0001	1.52	0.18
	120	0.001	1.15	0.06
	120	0.01	2.19	0.34
	140	0.0001	0.76	-0.12
	140	0.001	0.76	-0.12
	140	0.01	0.52	-0.28

Source: Output DTN: MO0311SPAEP MUT.000; halite divide ratio for dust.xls.

Implementation of Ionic Strength and Chloride Concentration Uncertainties—Quantifying and implementing uncertainties for the chemical parameters of ionic strength and chloride concentration are to be carried out as explained in the steps directly below. The two distributions for ionic strength and chloride concentration ([Cl⁻]) should be co-varied using same-scaled random uncertainty factor (i.e., the two parameters can use the same sampled distribution), as the ionic strength directly depends upon the often-dominant chloride concentration.

1. Look up the appropriate parameter value (ionic strength or [Cl⁻]) from the relevant TSPA-LA lookup table, for either dust deliquescence or seepage. Convert this value to

its $\log_{10}$ -base quantity; this becomes the value for which the subsequent distribution will be developed.

2. Create a uniform parameter uncertainty range that extends from the $\log_{10}$ -base quantity calculated in Step 1 by adding and subtracting the parameter binning uncertainty (Table 6.12-4 or 6.12-8) for each parameter.
3. Randomly choose a parameter value within this range (thereby producing a log uniform probability of occurrence) to obtain the $\log [\text{Cl}^-]$ or ionic strength that includes the binning uncertainty.
4. Combine the $[\text{Cl}^-]$ or ionic strength log value from Step 3 which includes the binning uncertainty with the model uncertainty by adding and subtracting the model uncertainty tabulated as a function of RH in Table 6.12-1. This will establish upper and lower bounds for the $\log [\text{Cl}^-]$ and ionic strength.
5. Randomly choose a parameter value within this range (thereby producing a log uniform probability of occurrence) to obtain the $\log [\text{Cl}^-]$ or ionic strength that includes both binning uncertainty and model variability.
6. Take the adjusted uncertainty log value and convert this back to nonlog units.

Implementation of Chloride–Nitrate Ratio Uncertainties—Quantifying uncertainties for the chemical parameter of chloride to nitrate concentration is to be carried out as explained in the steps below:

1. Using the $[\text{Cl}^-]$ and $[\text{NO}_3]$ concentrations from the lookup table determinations (without uncertainty), compute the chloride-to-nitrate ratio without uncertainty. Calculate the chloride to nitrate ratio from the appropriate TSPA-LA lookup table, either for dust deliquescence or seepage, then convert this value to its $\log_{10}$ -base quantity. This becomes the nominal value for which the subsequent distribution will be developed.
2. Create a uniform parameter uncertainty range that extends from the $\log_{10}$ -base quantity calculated in Step 1 by adding and subtracting the bin uncertainty from Table 6.12-4 or 6.12-8 to account for bin uncertainty.
3. Randomly choose a parameter value within this range (thereby producing a uniform probability of occurrence) to obtain a $\text{Cl}:\text{NO}_3$ that includes the binning uncertainty. Note the difference between this step and the nominal $\log \text{Cl}:\text{NO}_3$ ratio (Step 1). Call this difference delta because it will be used in Step 4 to adjust the theoretical log upper limit for $\text{Cl}:\text{NO}_3$. Delta can be a positive or negative value.
4. From the $\text{Cl}:\text{NO}_3$ halite divide molal ratio lookup table (Table 6.12-29 or 6.12-30), find the nominal theoretical upper limit as a function of bin, temperature, and $p\text{CO}_2$. Adjust this upper limit for binning uncertainty by adding the delta determined in Step 3.

5. Combine the $\text{Cl}:\text{NO}_3$ log value from Step 3, which includes the binning uncertainty, with the model uncertainty by adding and subtracting the log of the model uncertainty tabulated as a function of RH in Table 6.12-1. This will establish a lower and a preliminary upper bound for the log $\text{Cl}:\text{NO}_3$ ratio.
6. Compare the preliminary upper bound established in Step 5 with the theoretical upper bound established in Step 4. If the upper bound of Step 4 is more than the value of Step 5, then set the final log upper bound to equal the value of Step 5. If the value of Step 4 is less than the value of Step 5, use the theoretical upper limit of Step 4 as the final value for the log upper bound.
7. Sample randomly from the range of log $\text{Cl}:\text{NO}_3$ ratio established in Steps 5 and 6 to obtain a value that includes both binning and modeling uncertainties (i.e., log uniform distribution). If the preferred ratio is nitrate to chloride ($\text{NO}_3:\text{Cl}$) proceed with the negative value of this resulting $\log_{10}$ -base quantity. Convert this $\log_{10}$ -base quantity back to a ratio of nonlog units.

Calculation of Nitrate Concentration and Uncertainty—To obtain a consistent and correlated nitrate concentration value it must be calculated from the two previously determined chemical conditions of chloride concentration and chloride to nitrate ratio.

1. Take the value for the chloride concentration and divide it by the chloride to nitrate ratio, where both of these values have already been adjusted to their uncertainty ranges.

Implementation of pH Uncertainties—Quantifying and implementing uncertainties for the pH is to be carried out as explained in the steps directly below. This will yield a uniform distribution centered on the pH value initially selected from the TSPA-LA lookup table.

1. Choose the appropriate pH value from the relevant TSPA-LA lookup table (dust deliquescence or seepage). This will become the nominal pH value for a subsequent distribution to be developed for this parameter.
2. Create a uniform parameter uncertainty range that extends from the nominal pH in Step 1 by adding and subtracting the bin uncertainty from either Table 6.12-4 or 6.12-8.
3. Randomly select a value from the range established in Step 2 to produce a pH adjusted for binning uncertainty.
4. Create a uniform parameter uncertainty range that extends from the pH in Step 3, which includes binning uncertainty by adding and subtracting the model uncertainty of Table 6.12-1.
5. Randomly select a value from the range established in Step 4 to produce a pH adjusted for both binning and modeling uncertainty.

Implementation of Deliquescence Relative Humidity Point Uncertainties—There is uncertainty in the deliquescence relative humidity (DRH), the value of the relative humidity below which no stable aqueous solution exists. That is to say, at RH levels lower than those in the tables, stable aqueous solutions do not exist and therefore no values for solution composition parameters are given. The uncertainty range of the DRH point is given on Table 6.12-1.

The TSPA-LA dust deliquescence lookup tables provide, except for Bin 1, aqueous solution compositions down to values of RH that define the deliquescence point. Bin 1 is characterized by Na-CaNO₃ salts and a DRH is not predicted; this bin should be treated as having a DRH of 0 percent RH, that is, aqueous conditions would exist at all temperatures and RHs.

The TSPA-LA seepage evaporation lookup tables approach, but do not always predict the deliquescence RH point. When seepage chemistry is to be predicted, the conservative modeling decision of always having aqueous conditions should be made regardless of RH.

Quantifying and implementing uncertainties associated with the DRH point for dust leachate chemistries on the waste packages are to be carried out as explained in the steps below.

1. The DRH point is to be determined by selecting the appropriate nominal value from the TSPA-LA lookup table for dust deliquescence or seepage (the lowest RH point for a given bin selection subsequently referred to as DRH_{nominal}).
2. Add and subtract the amount of RH uncertainty found in Table 6.12-1 to the DRH_{nominal} to establish the upper and lower bounds of a DRH uncertainty range.
3. Randomly select a value from the range established in Step 2 between the estimated bounding values. This will yield the DRH adjusted to account for uncertainty.
4. For dust deliquescence, once the RH of the emplacement drift exceeds the value of $DRH_{\text{wUncertainty}}$, aqueous conditions are assumed to exist except for dust Bin 1 where aqueous conditions should always be assumed. Under seepage conditions, wet conditions should always be assumed. The composition of the aqueous solution that exists is taken from the suitable lookup table with the following rules:
  - a) If the $DRH_{\text{wUncertainty}}$ value is below that of the DRH in the lookup tables, then once the emplacement drift RH is at or just above $DRH_{\text{wUncertainty}}$, the chemical composition is taken as being that at the lookup table DRH until the drift RH reaches the next highest RH value given in the lookup table.
  - b) If the $DRH_{\text{wUncertainty}}$ value is above that of the DRH in the lookup table, then dry conditions exist until the emplacement drift RH equals or exceeds the value of $DRH_{\text{wUncertainty}}$. At this point, the aqueous composition at the DRH from the lookup table is used. At drift RH values above $DRH_{\text{wUncertainty}}$, the lookup table is to be accessed directly.

6.13 ENGINEERED BARRIER SYSTEM CHEMICAL ENVIRONMENT

The engineered barrier system (EBS) chemical environment analyses focus on a quantitative description of the pH, ionic strength (I), and major ionic and elemental compositions of waters in contact with the waste package and drip shield and the invert. The brines that form by evaporative concentration from the crown seepage over time can potentially affect localized corrosion rates on the waste package and drip shield, and influence radionuclide mobility in the invert. Corrosion of the Alloy-22 forming the waste package may lead to premature release of radionuclides from the waste form. Elemental ratios such as Cl:N are important in assessing the potential for localized corrosion of the waste package in the EBS environment (BSC 2004 [DIRS 169984], Figure 6-1; BSC 2004 [DIRS 169845]). Acidic or alkaline pH values of water in the invert can enhance the solubility of radionuclides. The ionic strength of water in the invert will control the mobility of colloidal material transporting sorbed radionuclides.

In addition, dust that accumulates on waste packages or drip shields during the operational and ventilation time periods may contain soluble salts, which will cause water condensation if the in-drift humidity is higher than the minimum deliquescent point of the salts. The resulting concentrated solution can potentially affect the degradation of the waste package outer barrier and drip shield.

This section summarizes the results of the P&CE model described in this document, establishing the magnitude and range of chemical variables in the processes involved, and establishing the foundation for the TSPA-LA modeling approach for the EBS environment.

Two terms, widely used in this document, are defined again here to ensure that the reader understands the material presented in this section. "Bin" is defined as a group of THC seepage model output waters with physical and chemical characteristics (Section 6.6.4), that fall within a single geochemical group as determined by chemical divides or precipitated minerals upon evaporation. A "bin history" is defined as the discretized version of the evolution curves (Section 6.6.6) of the five THC seepage model starting water compositions, for both invert and crown seepage waters, in which the water compositions at each time interval are mapped to the compositional bins to which they belong.

As calculated in Section 6.8.4, the quantifiable effects of Stainless Steel Type 316L active corrosion on seepage water for pH and ionic strength are insignificant at 100 percent relative humidity and negligible at 98 percent relative humidity. Based on these results and the results of the uncertainty calculations presented in Section 6.12.4, it has been concluded that active corrosion of the ground support will not appreciably influence the composition of the seepage waters in the drift.

To determine the most likely water chemistries for both the waste package surface and the invert over a given time interval, a time-integrated bin probability is calculated for both the crown seepage and dust leachate waters from the bin histories. This provides a quantitative probability of occurrence for a given "binned" water type over the time interval of interest, and enables determination of which water compositions and concentrations are likely to occur in a given period.

Figure 6.13-1 has been created from the bin history maps (Section 6.6.6) and other work prepared for model validation (Section 7.2). This work is documented in *Time integration20013.xls* (DTN: MO0312SPAPCESA.002). Figure 6.13-1 shows the bin history maps for each of the five waters in a color-coded scheme. Also calculated in this spreadsheet is the time-integrated bin probability for waters entering the crown of the drift and the invert. The probability is calculated by determining the relative percent of time each bin occurs for the five different waters. The relative weighting for a bin at a given time step is calculated by dividing the time step by the total length of the time interval examined. By totaling the relative weighting of the individual time steps according to bin, the percent of time the waters from each bin occur is calculated for each of the five different starting waters. This total is, for the specified time interval, the time-integrated probability of occurrence for each bin, for the five different waters entering the crown of the drift and the invert.

Source: Output DTN: MO0312SPAPCESA.002.

Figure 6.13-1. Color-Coded Bin History Maps Showing Differences Between Crown Seepage and Invert Wicking

The bin history maps show the composition of most-likely seepage waters—the liquid water existing closest to the drift in any given time step. They do not necessarily represent water present at the drift face. At early times (<~1,800 years), when temperatures exceed the boiling point of water at the drift wall, the vaporization barrier should prevent water from entering the drift. In these early time steps, the most proximal liquid water may be meters into the drift wall. Only after temperatures have cooled below boiling (96°C at the elevation of the repository) will the given compositions correspond to waters at the drift face.

The resulting time-integrated bin probabilities for the first 20,000 years after closure are shown in Tables 6.13-1 (crown seepage waters) and 6.13-2 (invert wicking waters), where each of the

five starting waters are equally likely to occur and the normalized values reflect the sum total of all five starting waters. These probabilities represent the percent of time that each bin water is expected to enter the drift at the given location. For instance, in the first 20,000 years, if W0 is the chosen starting water, Bin 3 water will be present at the drift crown for 1.12 percent of the time, or 224 years. However, since all five waters are equally probable, Bin 3 water will be present at the crown, on the average, for 0.22 percent of the time, or 44 years. These probabilities are only applicable for the time interval 0 to 20,000 years, as the bin occurrences are not randomly distributed through time (Figure 6.13-1).

Table 6.13-1. Time-Integrated Bin Probability for Any Given Crown Seepage Bin (20,000 Year Case)

Water	W0 %	W4 %	W5 %	W6 %	W7 %	Sum %	Norm %
Bin 1	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Bin 2	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Bin 3	1.12	0.00	0.00	0.00	0.00	1.12	0.22
Bin 4	2.62	1.00	1.00	1.00	1.50	7.12	1.42
Bin 5	0.56	1.87	1.00	0.00	0.50	3.93	0.79
Bin 6	25.82	0.00	0.00	1.50	0.00	27.32	5.46
Bin 7	31.75	26.48	32.01	0.25	45.25	135.74	27.15
Bin 8	12.50	31.03	12.50	12.50	12.50	81.02	16.20
Bin 9	0.00	12.50	13.00	39.75	12.50	77.75	15.55
Bin 10	0.00	0.25	13.24	45.00	0.00	58.49	11.70
Bin 11	25.63	26.88	27.25	0.00	27.75	107.50	21.50
Sum	100.00	100.00	100.00	100.00	100.00	500.00	100.00

Source: Output DTN: MO0312SPAPCESA.002.

NOTE: W0 through W7 refer to the THC seepage model outputs as listed in Section 4.1.3.1.

Table 6.13-2. Time-Integrated Bin Probability for Any Given Invert Wicking Seepage Bin (20,000 Year Case)

Water	W0 %	W4 %	W5 %	W6 %	W7 %	Sum %	Norm %
Bin 1	0.29	0.00	0.10	0.10	0.10	0.59	0.12
Bin 2	2.17	0.00	0.19	0.24	0.69	3.29	0.66
Bin 3	0.62	0.00	0.05	0.00	1.30	1.97	0.39
Bin 4	1.37	1.92	1.87	1.87	1.46	8.50	1.70
Bin 5	5.01	1.37	0.87	0.00	0.66	7.92	1.58
Bin 6	12.50	0.00	0.00	0.00	1.00	13.50	2.70
Bin 7	45.00	26.48	32.01	0.25	45.25	148.99	29.80
Bin 8	12.50	31.03	12.50	12.50	12.50	81.02	16.20
Bin 9	1.00	12.50	12.50	40.04	12.50	78.53	15.71
Bin 10	0.00	0.25	13.24	45.00	0.00	58.49	11.70
Bin 11	19.53	26.45	26.66	0.00	24.54	97.18	19.44
Sum	100.00	100.00	100.00	100.00	100.00	500.00	100.00

Source: Output DTN: MO0312SPAPCESA.002.

NOTE: W0 through W7 refer to the THC seepage model outputs as listed in Section 4.1.3.1.

The results in Table 6.13-1 show that for the drift crown, the probability of waters from Bins 1 and 2 coming in contact with the waste package and drip shield is zero. The bin waters most likely to be present as crown seepage through the critical time period (701 to 7,000 years), when the repository is cooling down, are Bins 4, 9, and 11, with small amounts of time with waters from Bins 5 and 6. For the invert, during 701 to 7,000 years, waters from Bins 4, 5, 9, and 11 are dominant, with small amounts of time when Bin 6 water is most likely. However, from 7,001 to 20,000 years at both the crown and the invert, waters from Bins 7 and 8 are the most likely bins, with Bin 10 waters also occurring in both the crown and the invert, and Bin 6 only in the crown. For periods beyond 20,000 years, only Bin 8 waters will be present. Only during the high-temperature period (from 51 to 700 years) do the more corrosive Bin 1, 2, and 3 waters potentially enter the repository, with Bin 3 water possibly occurring in the crown and the invert, and Bin 1 and 2 waters possibly occurring in the invert. This high temperature period is precisely the time when there is the least potential for liquid water to enter the drift, due to the heat energy generated within the waste packages.

These observations have been included in Table 6.13-3, which associates the bins with five general periods of repository time. These periods are associated with general thermal or operational constraints. They include the preclosure period (0 to 50 years), the boiling period (51 to 700 years), a hot period (701 to 2,000 years), a cool-down period (2,001 to 7,000 years), and a return to ambient period (7,001 to 20,000) years. Although the chemistry is similar, the hot and cool-down periods are generally separated by a short, chemically distinct period that is shown in the bin histories (Tables 6.6-8 through 6.6-12 and Figure 6.13-1) and the THC seepage results (Figures 6.6-20 through 6.6-29). It corresponds to the period in which the fractures in the drift wall start to rewet (Figures 6.6-2 through 6.6-4).

Table 6.13-3. Water Bins Associated with Different Periods in the Repository Thermal History

Water Location	0 to 50 years (Preclosure)	51 to 700 years (Boiling)	701 to 2,000 years (Hot)	2,001 to 5,000 years (Cool Down)	5,001 to 20,000 years (Return to Ambient)
Crown	4,7,10	3,4,5,6,9,11	4,5,6,9,11	6,9,11	6,7,8,9,10
Invert	4,7,10	1,2,3,4,5,9,11	4,5,6,9,11	6,9,11	6,7,8,9,10

NOTE: Bins marked in bold are the most likely for each period, based on Figure 6.13-1.

At the edges of the repository, the duration of the heat pulse will be much shorter. The net effect of this distance on the "center of repository" results that are reported in this section would be to shorten the boiling and hot periods and result in reaching the cool-down period sooner (Table 6.13-3 for the associated bins).

Additional time integrated probability calculations are done for the period beyond 20,000 years (archived in DTN: MO0312SPAPCESA.002) exactly as described for the 20,000-year case, with the upper bound changed to 35,024, 50,034, and 100,000 years. These calculations demonstrate that for times greater than 20,000 years, Bin 8 waters increasingly become the most likely water type. Only the probabilities calculated at 20,000 years, the regulatory time interval, are used throughout the remainder of this document.

In addition to the time integrated bin probabilities previously discussed, a second discrete probability distribution is also presented. This approach looks at the probability of the occurrence of the waters from any given bin at any given time.

As described in Section 6.6, the abstraction of the THC model incoming seepage waters resulted in the definition of eleven groups of waters based on water type. Single median waters were chosen from these groups (or bins) to represent the bin in the abstraction. Bin histories were developed to mimic the incoming water compositions predicted by the THC model to be the most likely waters to seep into the drift.

Because there were five THC model runs, each with a different starting water composition (w0, w4, w5, w6, and w7), five bin histories are mapped for the crown seepage and five bin histories are mapped for the invert seepage (Section 6.6.6). These five THC starting water compositions are determined to be equally probable. Therefore, each bin has a 0 percent, 20 percent, 40 percent, 60 percent, 80 percent, or 100 percent probability of occurring in the TSPA-LA model at any given time.

The bin probabilities are calculated for the crown and invert seepage for the time intervals defined in the bin histories. They are presented in Tables 6.13-4 and 6.13-5. Time intervals are approximated where noted in the tables. Approximations have been made where time intervals did not exactly match between bin histories.

Table 6.13-4. Bin Probabilities for Crown Seepage as a Function of Time

Start (yr)	End (yr)	Bin 1	Bin 2	Bin 3	Bin 4	Bin 5	Bin 6	Bin 7	Bin 8	Bin 9	Bin 10	Bin 11
0.0	30.5	—	—	—	20%	—	—	60%	—	—	20%	—
30.5	52.0	—	—	—	—	20%	—	—	—	20%	—	60%
52.0	54.0	—	—	—	—	20%	—	—	—	20%	—	60%
54.0	57.5	—	—	—	—	—	20%	—	—	20%	—	60%
57.5	67.5	—	—	—	—	—	20%	—	—	20%	—	60%
67.5	87.5	—	—	—	—	20%	—	—	—	20%	—	60%
87.5	125.0	—	—	—	—	20%	—	—	—	20%	—	60%
125.0	175.0	—	—	—	20%	—	—	—	—	20%	—	60%
175.0	225.0	—	—	—	20%	—	—	—	—	20%	—	60%
225.0	275.0	—	—	20%	—	—	—	—	—	20%	—	60%
275.0	325.0	—	—	20%	—	20%	—	—	—	20%	—	40%
325.0	375.0	—	—	20%	20%	—	—	—	—	20%	—	40%
375.0	450.0	—	—	20%	20%	—	—	—	—	20%	—	40%
450.0	550.0	—	—	—	40%	20%	20%	—	—	20%	—	—
550.0	625.0	—	—	—	40%	20%	—	—	—	20%	—	20%
625.0	675.0	—	—	—	—	40%	—	—	—	20%	—	40%
675.0	725.0	—	—	—	—	—	—	—	—	20%	—	80%
725.0	775.0	—	—	—	—	—	—	—	—	20%	—	80%
775.0	900.0	—	—	—	—	—	—	—	—	20%	—	80%
900.0	1,100.0	—	—	—	—	—	—	—	—	20%	—	80%
1,100.0	1,300.0	—	—	—	—	—	—	—	—	20%	—	80%
1,300.0	1,500.5	—	—	—	—	—	—	—	—	20%	—	80%
1,500.5	1,701.0	—	—	—	—	—	—	—	—	20%	—	80%
1,701.0	1,901.0	—	—	—	—	40%	20%	—	—	—	—	40%
1,901.0	2,101.0	—	—	—	80%	—	—	—	—	—	—	20%
2,101.0	2,301.0	—	—	—	—	—	—	—	—	20%	—	80%
2,301.0	2,701.5	—	—	—	—	—	—	—	—	20%	—	80%
2,701.5	4,002.5	—	—	—	—	—	—	—	—	20%	—	80%
4,002.5	6,003.5	—	—	—	—	—	—	—	—	20%	—	80%
6,003.5	8,505.0	—	—	—	—	—	20%	—	—	80%	—	—
8,505.0	11,289.0 ^a	—	—	—	—	—	20%	40%	—	—	40%	—
11,289.0 ^a	13,791.0 ^a	—	—	—	—	—	—	80%	—	—	20%	—
13,791.0 ^a	17,511.5	—	—	—	—	—	—	60%	20%	—	20%	—
17,511.5	35,023.5	—	—	—	—	—	—	—	100%	—	—	—
35,023.5	100,000.0	—	—	—	—	—	—	—	100%	—	—	—

Source: Table 6.13-1.

^a Approximated time interval cutoff to accommodate all bin histories.

Table 6.13-5. Bin Probabilities for Invert Seepage as a Function of Time

Start (yr)	End (yr)	Bin 1	Bin 2	Bin 3	Bin 4	Bin 5	Bin 6	Bin 7	Bin 8	Bin 9	Bin 10	Bin 11
0.0	30.5	—	—	—	20%	—	—	60%	—	—	20%	—
30.5	52.0	—	—	—	—	20%	—	—	—	20%	—	60%
52.0	54.0	—	—	—	—	—	—	—	—	20%	—	80%
54.0	57.5	—	—	—	—	—	—	—	—	20%	—	80%
57.5	67.5	—	40%	40%	20%	—	—	—	—	—	—	—
67.5	87.5	60%	—	—	20%	—	—	—	—	—	—	20%
87.5	125.0	20%	60%	—	—	—	—	—	—	—	—	20%
125.0	175.0	—	20%	—	80%	—	—	—	—	—	—	—
175.0	225.0	—	20%	—	80%	—	—	—	—	—	—	—
225.0	275.0	—	20%	—	20%	40%	—	—	—	20%	—	—
275.0	325.0	—	20%	20%	60%	—	—	—	—	—	—	—
325.0	375.0	—	20%	20%	40%	20%	—	—	—	—	—	—
375.0	450.0	—	20%	20%	20%	20%	—	—	—	20%	—	—
450.0	550.0	—	40%	—	60%	—	—	—	—	—	—	—
550.0	625.0	—	—	40%	40%	20%	—	—	—	—	—	—
625.0	675.0	—	—	20%	40%	20%	—	—	—	20%	—	—
675.0	725.0	—	—	—	40%	20%	—	—	—	20%	—	20%
725.0	767.0 ^a	—	—	—	40%	20%	—	—	—	20%	—	20%
767.0 ^a	792.0 ^a	—	—	—	20%	20%	—	—	—	20%	—	40%
792.0 ^a	900.0	—	—	—	20%	20%	—	—	—	20%	—	40%
900.0	1,100.0	—	—	—	—	20%	20%	—	—	20%	—	40%
1,100.0	1,300.0	—	—	—	—	20%	—	—	—	20%	—	60%
1,300.0	1,500.5	—	—	—	—	20%	—	—	—	20%	—	60%
1,500.5	1,701.0	—	—	—	—	20%	—	—	—	20%	—	60%
1,701.0	1,901.0	—	—	—	—	20%	—	—	—	20%	—	60%
1,901.0	2,101.0	—	—	—	—	—	—	—	—	40%	—	60%
2,101.0	2,301.0	—	—	—	—	—	—	—	—	20%	—	80%
2,301.0	2,701.5	—	—	—	—	—	—	—	—	20%	—	80%
2,701.5	4,002.5	—	—	—	—	—	—	—	—	20%	—	80%
4,002.5	6,003.5	—	—	—	—	—	—	—	—	20%	—	80%
6,003.5	8,505.0	—	—	—	—	—	20%	—	—	80%	—	—
8,505.0	11,228.3 ^a	—	—	—	—	—	—	60%	—	—	40%	—
11,228.3 ^a	13,730.3 ^a	—	—	—	—	—	—	80%	—	—	20%	—
13,730.3 ^a	17,511.5	—	—	—	—	—	—	60%	20%	—	20%	—
17,511.5	35,023.5	—	—	—	—	—	—	—	100%	—	—	—
35,023.5	100,000.0	—	—	—	—	—	—	—	100%	—	—	—

Source: Table 6.13-1.

^a Approximated time interval cutoff to accommodate all bin histories.

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 (Ttptll) (BSC 2004 [DIRS 169856]). 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

temperatures ranging from 40°C to 100°C, fugacities of CO₂ from 10⁻⁴ to 10⁻² atmospheres, and relative humidity in the drift from 0 to 100 percent.

Figures 6.13-2 through 6.13-12 show the seepage evaporation lookup tables for each of the 11 bins. These figures are meant only to illustrate the general output trends. The actual values are provided in the specific lookup tables listed in Table 6.9-6. For each bin, there are nine evaporation runs represented, one for each combination of temperature (40°C, 70°C, and 100°C) and CO₂ fugacity (10⁻⁴, 10⁻³, and 10⁻² bar).

Source: Output DTN: MO0304SPACPSLT.000.

Figure 6.13-2. Aqueous Composition Predictions Versus Relative Humidity for All Seepage Evaporation Lookup Tables for Bin 1 (IS = Ionic Strength)

Source: Output DTN: MO0304SPACPSLT.000.

Figure 6.13-3. Aqueous Composition Predictions Versus Relative Humidity for All Seepage Evaporation Lookup Tables for Bin 2 (IS = Ionic Strength)

Source: Output DTN: MO0304SPACPSLT.000.

Figure 6.13-4. Aqueous Composition Predictions Versus Relative Humidity for All Seepage Evaporation Lookup Tables for Bin 3 (IS = Ionic Strength)

Source: Output DTN: MO0304SPACPSLT.000.

Figure 6.13-5. Aqueous Composition Predictions Versus Relative Humidity for All Seepage Evaporation Lookup Tables for Bin 4 (IS = Ionic Strength)

Source: Output DTN: MO0304SPACPSLT.000.

Figure 6.13-6. Aqueous Composition Predictions Versus Relative Humidity for All Seepage Evaporation Lookup Tables for Bin 5 (IS = Ionic Strength)

Source: Output DTN: MO0304SPACPSLT.000.

Figure 6.13-7. Aqueous Composition Predictions Versus Relative Humidity for All Seepage Evaporation Lookup Tables for Bin 6 (IS = Ionic Strength)

Source: Output DTN: MO0304SPACPSLT.000.

Figure 6.13-8. Aqueous Composition Predictions Versus Relative Humidity for All Seepage Evaporation Lookup Tables for Bin 7 (IS = Ionic Strength)

Source: Output DTN: MO0304SPACPSLT.000.

Figure 6.13-9. Aqueous Composition Predictions Versus Relative Humidity for All Seepage Evaporation Lookup Tables for Bin 8 (IS = Ionic Strength)

Source: Output DTN: MO0304SPACPSLT.000.

Figure 6.13-10. Aqueous Composition Predictions Versus Relative Humidity for All Seepage Evaporation Lookup Tables for Bin 9 (IS = Ionic Strength)

Source: Output DTN: MO0304SPACPSLT.000.

Figure 6.13-11. Aqueous Composition Predictions Versus Relative Humidity for All Seepage Evaporation Lookup Tables for Bin 10 (IS = Ionic Strength)

Source: Output DTN: MO0304SPACPSLT.000.

Figure 6.13-12. Aqueous Composition Predictions Versus Relative Humidity for All Seepage Evaporation Lookup Tables for Bin 11 (IS = Ionic Strength)

The combination of the nine individual lookup tables for each bin represents a response surface for the chemistry in that bin, so they suggest the potential ranges of outputs for the ranges of inputs simulated. These figures provide the entire range of values for each compositional variable. However, in the TSPA-LA simulations, the potential range of values is constrained to a single evolution path for each variable by the choice of $p\text{CO}_2$ and temperature. The predicted relative humidity will further constrain the possible value of each parameter to a narrow range on each curve.

For example, the Bin 1 results shown in Figure 6.13-2 indicate that pH values could vary from 8 or 9 to 3.5 for the ranges of temperature, CO_2 fugacity, and relative humidity modeled. However, according to the bin maps in Section 6.6.6, Bin 1 water only occurs in the invert between 57.5 years and 125 years. During this period, the temperature will be high and the CO_2 fugacity and relative humidity will be relatively low. The most-likely Bin 1 output values used in the TSPA-LA will correspond to those predicted at low relative humidity for the high-temperature, low- CO_2 fugacity simulation (01c4tle). The pH curve that corresponds to this case in Figure 6.13-2 is that with the highest pH values at a relative humidity of less than 35 percent. Consequently, if the relative humidity is less than 60 percent during this time period, which is reasonable, then the most likely pH range for TSPA-LA Bin 1 output is approximately 5 to 6, a much smaller range than the pH response surface represented in Figure 6.13-2.

Figure 6.13-13 displays the all-bin response surface for two molar ratios: Cl/NO_3 which is potentially important to corrosion, and $(\text{Cl}+\text{F})/(\text{NO}_3+\text{SO}_4)$, which provides information on additional ions that potentially inhibit corrosion. As is the case for the response surfaces for the individual components displayed in the previous figures in this section, the ranges for the ratios relevant to the TSPA-LA in any given time step are much smaller than the ranges plotted. In other words, many of the points plotted in Figure 6.13-13 (perhaps a majority based on an extrapolation of the analysis in the previous paragraph) have a TSPA-LA probability of occurrence that approaches zero.

Source: Output DTN: MO0304SPACPSLT.000.

Figure 6.13-13. Selected Aqueous Molal Ratios Useful for Corrosion Analysis Versus Relative Humidity for All Seepage Evaporation Lookup Tables for All Bins

6.13.1.3 Evaporative Brine Precipitate Mineralogy and Chemical Divide Phenomena

Each lookup table developed in Section 6.9 has an associated precipitating mineral assemblage. Mineral precipitation as a function of relative humidity and degree of evaporative concentration is presented for each individual lookup table in Appendix B. Table 6.13-6 summarizes the characteristic mineral assemblages for each of the 11 bins.

Table 6.13-6. Summary Table of Precipitating Minerals in Each of the Eleven Bins

Bin	Precipitating Minerals at the Start of EQ6 Runs	Additional Precipitating Minerals (Roman Numerals Represent the Precipitation Sequence)	Occurrence Notes
Bin 1	SiO _{2(am)} , Stellerite	Fluorite (I), Calcite (II), Anhydrite (III), Sepiolite (IV), Halite (V), Ca(NO ₃) ₂ (VI _a), Ca(NO ₃) ₂ ·3H ₂ O (VI _b), Ca(NO ₃) ₂ ·4H ₂ O (VI _c)	Sepiolite does not form at $p\text{CO}_2 = 10^{-2}$; calcium nitrates are strongly temperature dependant; a = 100°C; b = 70°C; c = 40°C.
Bin 2	SiO _{2(am)} , Stellerite	Calcite (I), Fluorite (II), Anhydrite (III), Sepiolite (IV), Halite (V), Soda Niter (VI)	Soda niter only forms at 40°C.
Bin 3	Stellerite, SiO _{2(am)}	Fluorite (I), Calcite (II), Anhydrite (III), Sepiolite (IV), Halite (V), Sylvite (VI), Niter (VII)	SiO _{2(am)} in one lookup table did not form at the start of the run; niter only forms at 40°C.
Bin 4	SiO _{2(am)} , Stellerite	Calcite (I), Fluorite (II), Anhydrite (III), Sepiolite (IV), Phillipsite (V), Glauberite (VI), Halite (VII), Pentasalt (VIII), Erionite (IX), Niter (X)	Zeolite minerals evolve in this bin in the following general manner: stellerite to phillipsite to erionite; niter does not show up in the 100°C-simulations tables; erionite does not show up in the 40°C modeling runs.
Bin 5	SiO _{2(am)} , Stellerite, Fluorite	Calcite (I), Sepiolite (II), Glauberite (III), Thenardite (IV), Erionite (V), Halite (VI), Syngenite (VII), Niter (VIII)	Syngenite does not form at 100°C; niter only forms in the 40°C, $p\text{CO}_2 = 10^{-4}$ modeling runs.
Bin 6	Stellerite, Calcite, Sepiolite	SiO _{2(am)} (I), Fluorite (II), Erionite (III), Thenardite (IV), Halite (V), Arcanite (VI), Natrite (VII _a), Nahcolite (VII _b), [Pirssonite, Burkeite, Trona] (VII _c)	Calcite and sepiolite do not precipitate at the start of the run in one model simulation (06c2t4e); natrite does not form at 40°C; nahcolite does not form at 100°C or at $p\text{CO}_2 = 10^{-4}$; burkeite, pirssonite and trona only form at 40°C and $p\text{CO}_2 = 10^{-4}$.
Bin 7	Calcite, Sepiolite, Stellerite	SiO _{2(am)} (I), Fluorite (II), Erionite (III), Thenardite (IV), Halite (V), Arcanite (VI), Natrite (VII _a), Nahcolite (VII _b), [Pirssonite, Burkeite, Trona] (VII _c)	Calcite and sepiolite do not precipitate at the start of the run in one model simulation (07c2t4e); stellerite does not precipitate at start of run in two of the three 100°C runs; natrite does not form at 40°C; nahcolite does not form at 100°C or at $p\text{CO}_2 = 10^{-4}$; burkeite, pirssonite and trona only form at 40°C and $p\text{CO}_2 = 10^{-4}$.
Bin 8	Calcite, Sepiolite	Stellerite (I), SiO _{2(am)} (II), Erionite (III), Fluorite (IV), Natrite (V _a), Nahcolite (V _b), [Pirssonite, Trona, Burkeite, Niter] (V _c), Thenardite (VI), Halite (VII), Arcanite (VIII)	Sepiolite does not form at the start in one model run (08c2t4e); stellerite does not form at all in three modeling runs; natrite does not form at 40°C, nahcolite does not form at 100°C or at $p\text{CO}_2 = 10^{-4}$; burkeite, pirssonite, niter and trona only form at 40°C and $p\text{CO}_2 = 10^{-4}$. When these 4 minerals form, thenardite does not.
Bin 9	Stellerite	Calcite (I), Sepiolite (II), SiO _{2(am)} (III), Fluorite (IV), Erionite (V), Villiaumite (VI), Natrite (VII _a), [Nahcolite, Sellaite, Cryolite] (VII _b), [Trona, Burkeite] (VII _c), Halite (VIII), Arcanite (IX)	Calcite does not form in two model runs (09c2t4e, 09c2t7e); natrite does not form at 40°C, nahcolite does not form at 100°C or at $p\text{CO}_2 = 10^{-4}$; arcanite does not form at 100°C; sellaite only appears at $p\text{CO}_2 = 10^{-2}$; cryolite, burkeite, and trona only form at 40°C and $p\text{CO}_2 = 10^{-4}$; nahcolite, trona, burkeite, niter, sellaite and cryolite only form when natrite does not. Trona and burkeite form when natrite and nahcolite do not.

Table 6.13-6. Summary Table of Precipitating Minerals in Each of the Eleven Bins (Continued)

Bin	Precipitating Minerals at the Start of EQ6 Runs	Additional Precipitating Minerals (Roman Numerals Represent the Precipitation Sequence)	Occurrence Notes
Bin 10	Calcite, Sepiolite	Stellerite (I), SiO _{2(am)} (II), Fluorite (III), Erionite (IV), Natrite (V _a), [Nahcolite, Sellaite, Cryolite] (V _b), [Trona, Burkeite, Niter] (V _c), Thenardite (VI), Villiaumite (VII) Arcanite (VIII), Halite (IX)	Sepiolite does not form at the start in one model run (10c4t1e); natrite does not form at 40°C; nahcolite does not form at 100°C or at $p\text{CO}_2 = 10^{-4}$, sellaite and cryolite only appear at $p\text{CO}_2 = 10^{-2}$; nahcolite, trona, burkeite, niter, sellaite and cryolite only form when natrite does not; trona, burkeite and niter only form when thenardite does not.
Bin 11	Fluorite, SiO _{2(am)} , Stellerite, Sepiolite	Calcite (I), Erionite (II), Villiaumite (III), Thenardite (IV _a), [Burkeite, Trona, Niter] (IV _b), Natrite (V _a), [Sellaite, Cryolite, Nahcolite] (V _b), [Sellaite, Nahcolite], (V _c), Nahcolite (V _d), Halite (VI), Arcanite (VII)	Sepiolite does not form at the start in two model runs (11c2t7e, 11c2t4e); calcite does not form in some model runs (11c2t4e, 11c4t1e, and 11c2t7e); burkeite, trona and niter only form when thenardite and natrite do not form; V _c and V _b only form when no calcite is present.

Source: Output DTN: MO0312SPAPCESA.002.

Based on the discussion of chemical divides in Section 6.2, an analysis of the lookup table mineralogy is provided in the following paragraphs, linking each of the bins to the precipitation of a particular sequence of minerals. The analysis is performed by extracting the mineral data from the EQ6 output files listed on Table 6.9-5 into *11 bin mineral assemblage.xls* using GETEQDATA software. This spreadsheet is archived in DTN: MO0312SPAPCESA.002. Within the spreadsheet, a simplified paragenetic sequence is constructed for each bin based on the order of mineral appearance, the temperature, and $p\text{CO}_2$ of each evaporated brine. This worksheet is the source of the information found on Table 6.13-6.

Using the information in Table 6.13-6, Figure 6.13-14 is constructed to illustrate which precipitating minerals control the trajectory of brine evolution as the seepage waters are evaporated.

*Previously Precipitating Minerals: Calcite, Fluorite, Sepiolite, Steffertite, Eriolite, $\text{SiO}_2(\text{am})$

*Bin 5 and Bin 7 do not tie directly to a precipitating mineral that defines the bin.
The items listed are the binning criteria that differentiate the two bins; see Table 6.6.5-3.

Figure 6.13-14. Flow Diagram Showing Some of the Precipitating Minerals Associated with Each of the 11 Seepage Bins

Although not directly equivalent to the classical chemical divides, as shown by Drever (1988 [DIRS 118564], p. 236) (Figure 6.2-1), Figure 6.13-14 does show the mineral phases that precipitate as the THC seepage waters evaporate, and that are associated with the 11 Bins. The presence or absence of anhydrite in the precipitated mineral assemblage separates the evaporative brine evolution of Bins 1 through 4 from Bins 5 through 11. Combined with the comparative pH results of all bins shown in Figures 6.13-15 and 6.13-16, three major groupings of brine chemistry and mineral precipitation can be seen, where not only the presence or absence of anhydrite, but the presence or absence of glauberite is associated with the distribution of the pH. In general, the sequencing of natrite, thenardite, and villiaumite characterizes the evolution of Bins 6 through 11. Bins 1 through 3 are characterized by early precipitation of halite and Bins 4 and 5 by the precipitation of glauberite. Bins 6 and 7 are a result of the binning criterion shown in Figure 6.13-14. In no cases do any calcium chloride, magnesium chloride, or calcium-magnesium chloride minerals, such as bischofite and tachyhydrite, precipitate.

Source: Output DTN: MO0312SPAPCESA.002.

Figure 6.13-15. Range of pH Versus Relative Humidity for the Seepage Evaporation Lookup Tables Representing Bins 3 through 11

Source: Output DTN: MO0312SPAPCESA.002.

Figure 6.13-16. Range of pH Versus Relative Humidity for the Seepage Evaporation Lookup Tables Representing Bins 1 and 2

6.13.2 Engineered Barrier System Dust Deliquescence Chemistry

Section 6.10 describes the development of lookup tables that represent the chemical compositions of dust leachate and brines forming by deliquescence on the waste package and drip shield surfaces. Appendix C contains figures for each individual lookup table that show the various chemical parameters as a function of relative humidity and concentration factor as well as the results of any individual lookup tables. The combined results from all lookup tables are discussed in the following paragraphs. Section 6.13.2.1 describes the distribution of starting waters and other initial modeling constraints that should be imposed on the results. Section 6.13.2.2 discusses what the dust leachate lookup tables represent and the ranges of outputs associated with these lookup tables.

6.13.2.1 Engineered Barrier System Dust Deliquescence Chemistry Constraints

When seepage into the repository does not occur, deliquescence of salts in dust deposited on the waste package and drip shield will control the chemistry of in-drift waters that affect corrosion. As shown on Table 6.10-6, the six dust leachate bins have a discrete probability of occurrence. The bin probabilities listed in Table 6.10-6 will serve as the likely distribution of waters formed by deliquescence (equivalent to assigning an equal probability of occurrence to all sampled waters; Assumption 5.2.1). To determine the value for $p\text{CO}_2$ in the drift, it is necessary to utilize a $p\text{CO}_2$ lookup table. As stated in Section 6.13.1.1, the probability for any given $p\text{CO}_2$ lookup table is tied to the probability of the starting water associated with that table. In the absence of seepage, each of the five lookup tables is given an equal probability of occurrence. These lookup tables are provided in Section 6.7.2.1 (Tables 6.7-1 through 6.7-5).

Figure 6.13-17 shows the H_2O vapor pressure curves associated with the activity of water (or RH) for all lookup tables at or above 100°C . Also plotted (orange line) is the pressure that is reported by the THC seepage model for in-drift pressures through time (0.89 bars; *THC CO2 GAS& TEMP COMPARE.xls* archived in output DTN: MO0308SPACO2GL.001, developed in Section 6.7). The intersection of these two values indicates the maximum value of water activity at which aqueous solutions can deliquesce on waste packages, given the drift pressure conditions. Essentially, any temperature and pressure condition above the orange line will not be able to sustain liquid water. These conditions indicate that there is no liquid water in the drift above 140°C , and limited liquid water at 120°C (water present below 44 percent RH) and 100°C (water present below 88 percent RH). However, uncertainties in the deliquescence relative humidity may shift the endpoints in these curves, so the possibility of liquid water at somewhat higher temperatures cannot be ruled out.

Source: Output DTN: MO0310SPAPCELA.002.

Figure 6.13-17. Range of H_2O Vapor Pressure Versus Activity of Water Resulting in Wet Conditions for All Dust Leachate Lookup Tables at or above 100°C

In-drift temperatures and relative humidity are calculated in *Multiscale Thermohydrologic Model* (BSC 2004 [DIRS 169565]). The model presented here is generalized, in which its results are discussed in terms of ranges.

6.13.2.2 Engineered Barrier System Dust Deliquescence Chemistry Response Surface Ranges

The set of dust leachate lookup tables developed and described in Section 6.10 are combined into one large lookup table to assess the overall ranges of model outputs. This combined lookup table, which is documented in DTN: MO0310SPAPCELA.002, defines six multidimensional response surfaces, one for each of the representative dust bin waters. From these response surfaces, the model outputs can be interpolated for temperatures ranging from 40°C to 140°C , fugacities of CO_2 from 10^{-4} to 10^{-2} atmospheres, and relative humidity from 0 to 100 percent.

Figures 6.13-18 through 6.13-23 show the water chemistries contained in the dust leachate lookup tables for each of the six bins. These figures are meant only to illustrate the general output trends. The actual values are provided in the specific lookup tables listed in Table 6.10-14. For each bin, there are fifteen evaporation runs represented, one for each

combination of temperature (40°C, 70°C, 100°C, 120°C, and 140°C) and CO₂ fugacity (10⁻⁴, 10⁻³, and 10⁻² bar).

Source: Output DTN: MO0310SPAPCELA.002.

Figure 6.13-18. Aqueous Composition Predictions Versus Relative Humidity for All Dust Leachate Lookup Tables for Bin 1 (IS = Ionic Strength)

Source: Output DTN: MO0310SPAPCELA.002.

Figure 6.13-19. Aqueous Composition Predictions Versus Relative Humidity for All Dust Leachate Lookup Tables for Bin 2 (IS = Ionic Strength)

Source: Output DTN: MO0310SPAPCELA.002.

Figure 6.13-20. Aqueous Composition Predictions Versus Relative Humidity for All Dust Leachate Lookup Tables for Bin 3 (IS = Ionic Strength)

Source: Output DTN: MO0310SPAPCELA.002.

Figure 6.13-21. Aqueous Composition Predictions Versus Relative Humidity for All Dust Leachate Lookup Tables for Bin 4 (IS = Ionic Strength)

Source: Output DTN: MO0310SPAPCELA.002.

Figure 6.13-22. Aqueous Composition Predictions Versus Relative Humidity for All Dust Leachate Lookup Tables for Bin 5 (IS = Ionic Strength)

Source: Output DTN: MO0310SPAPCELA.002.

Figure 6.13-23. Aqueous Composition Predictions Versus Relative Humidity for All Dust Leachate Lookup Tables for Bin 6 (IS = Ionic Strength)

The combination of the 15 individual lookup tables for each bin represents a response surface for the chemistry in that bin, so they suggest the potential ranges of outputs for the ranges of inputs simulated. These figures provide the entire range of values for each compositional variable, but in the TSPA-LA simulations, the potential range of values are constrained by the choice of $p\text{CO}_2$ and temperature to a single evolution path for each variable. The predicted relative humidity will further constrain the possible value of each parameter to a narrow range on each curve.

For example, the Bin 1 results shown in Figure 6.13-18 indicate that the range in possible pH values is from 6.3 to 8 in the initial waters, up to 10 for specific values of temperature, CO_2 fugacity, and relative humidity modeled. However, according to the bin distribution in Section 6.10.5.3.2 (Table 6.10-6), Bin 1 water only occurs about 5.8 percent of the time. The most likely bin (Bin 5) occurs about 44.2 percent of the time. The range of pH covered by this bin is 8 to 11.5, as shown on Figure 6.13-23.

Figure 6.13-24 displays the all-dust bin response surface for the two molar ratios Cl/NO_3 and $(\text{Cl}+\text{F})/(\text{NO}_3+\text{SO}_4)$. As was the case with the seepage waters, the ranges for these ratios that are relevant to the TSPA-LA may be smaller than the ranges plotted.

Source: Output DTN: MO0310SPAPCELA.002.

Figure 6.13-24. Selected Aqueous Molal Ratios Versus Relative Humidity for All Dust Leachate Lookup Tables for All Bins

6.13.2.3 Dust Leachate Evaporative Brine Precipitate Mineralogy and Chemical Divide Phenomena

Each lookup table developed in Section 6.10 has associated with it a precipitating mineral assemblage. Mineral precipitation as a function of relative humidity and degree of evaporative concentration is presented for each individual lookup table in Appendix C. Table 6.13-7 summarizes the characteristic mineral assemblages for each of the six bins.

Based on the discussion of chemical divides in Section 6.2, an analysis of the lookup table mineralogy is provided below, linking each of the six bins to the precipitation of a particular sequence of minerals. The analysis is performed by extracting the mineral data from the EQ6 output files listed on Table 6.10-12 into *Modified Dust Mineral Assemblage Spreadsheet.xls* using GETEQDATA. This spreadsheet is archived in DTN: MO0310SPAPCELA.002. Within the spreadsheet, a simplified paragenetic sequence is constructed for each bin based on the order of mineral appearance, the temperature, and $p\text{CO}_2$ of each evaporated brine. This worksheet is the source of the information found on Table 6.13-7.

Using the information on Table 6.13-7, Figure 6.13-25 has been constructed to provide an understanding as to which precipitating minerals are associated with the trajectory of brine evolution as the dust leachate waters are evaporated.

Figure 6.13-25. Flow Diagram Showing Some of the Precipitating Minerals Associated with Each of the 6 Dust Leachate Brine Evaporation Bins

Table 6.13-7. Summary Table of Precipitating Minerals in Each of the Six Dust Leachate Evaporation Bins

Bin	Precipitating Minerals at the Start of EQ6 Runs	Additional Precipitating Minerals (Numerals Represent Precipitation Sequence) [Brackets Represent Limited Precipitation]	Occurrence Notes
Bin 1	Calcite, Sepiolite, [Brucite]	Anhydrite (I), Sellaite (II), Halite (III), [Fluorite (IV)], Huntite (V), Niter (VI), Soda Niter (VII), KBr (VIII), [Ca (NO ₃) ₂]	Brucite forms only at or above 100°C and $p\text{CO}_2 = 10^{-3}$ or higher; calcite always precipitates at the start of a run except at $p\text{CO}_2 = 10^{-2}$ and temperature = 100°C; sepiolite always forms first or second in sequence for all $p\text{CO}_2$ and temperature conditions; fluorite only forms at 100°C or higher at $p\text{CO}_2 = 10^{-4}$; Ca(NO ₃) ₂ only forms in one model simulation (d1c4t14.6o).
Bin 2	Calcite, [Brucite]	Sepiolite (I), Anhydrite(II), Sellaite (III) [Fluorite (IV)], Huntite (V), Glauberite (VI), Pentasalt (VII), Halite (VIII), [Sylvite (IX)], Niter (X), KBr (XI)	Calcite always precipitates first in sequence for all $p\text{CO}_2$ and temperature conditions; sepiolite always forms either second or third in sequence; brucite forms only at or above 100°C and $p\text{CO}_2$ of 10^{-3} or higher. Niter and KBr always form late in sequence when present; fluorite only forms at $p\text{CO}_2 = 10^{-4}$ and temperatures = 100°C or higher; pentasalt never forms above 100°C; sylvite only forms at 140°C; anhydrite usually forms after calcite or after sepiolite in sequence.
Bin 3	Calcite, [Brucite]	Sepiolite (I), Sellaite (II), Fluorite (III), Huntite (IV), Arcanite (V), Thenardite (VI), [Nahcolite (VIIa), Hallite (VIIa)], [Thermonatrite (VIIb), Hallite (VIIb)], [Natrium (VIIc), Hallite (VIIc)], [Niter (VIIId), KBr (VIIId)]	Calcite always precipitates first in sequence for all $p\text{CO}_2$ and temperature conditions; sepiolite always forms either second or third in sequence; sellaite usually forms after sepiolite; brucite forms only at or above 100°C and $p\text{CO}_2 = 10^{-3}$ or higher; niter and KBr form late in sequence when present; thermonatrite only precipitates at 100°C; villiaumite, pirssonite and burkeite precipitate in one calculation each.
Bin 4	Calcite, [Brucite]	Sepiolite (I), Anhydrite (II), [Sellaite (III)], [Huntite (IV)], [Fluorite (V)], Glauberite (VI), Halite (VII), Niter (VIII), Soda Niter (IX), KBr (X)	The first few minerals to precipitate at 70°C or higher usually are calcite (or brucite), sepiolite, anhydrite (or sellaite); brucite forms only at or above 100°C and $p\text{CO}_2 = 10^{-3}$ or higher; niter and KBr always form late in sequence when present; fluorite only precipitates at $p\text{CO}_2 = 10^{-4}$ and temperatures at 100°C or above.
Bin 5	Calcite, [Brucite]	Sepiolite(I), Fluorite (II), Sellaite (III), Glauberite (IV), Thenardite (V), Halite (VI), Niter (VII), KBr (VIII), [Soda Niter (IXa), Darapskite (IXb)]	Calcite always precipitates at the start of a run, usually followed by sepiolite; commonly, after sepiolite forms, fluorite, sellaite, and glauberite form; brucite forms only at or above 100°C and $p\text{CO}_2 = 10^{-3}$ or higher; niter, KBr, soda niter, and darapskite form late in sequence when they are present.
Bin 6	Calcite, [Brucite]	Sepiolite (I), SiO _{2(am)} (II), Fluorite (III), Arcanite (IV), [Villiaumite (V), Thenardite (VI), Natrite (VII), Nahcolite (VIII), Halite (IX), Pirssonite (X), Sylvite (XI), Niter (XII), KBr (XIII)]	Calcite usually precipitates first in sequence and sepiolite second; after sepiolite precipitates, either fluorite, arcanite, or SiO _{2(am)} usually form; brucite forms only at or above 120°C and $p\text{CO}_2 = 10^{-3}$ or higher; halite never forms above 100°C; nahcolite only forms at 40°C; sylvite never forms above 100°C; niter never forms above 70°C.

Source: Output DTN: MO0310SPAPCELA.002.

Although not directly equivalent to Figure 6.2-1 in its chemical divides, Figure 6.13-25 does show the mineral phases associated with the brine evolution of the dust leachate waters as they are associated with the six leachate evaporation bins. The presence or absence of anhydrite divides Bins 1, 2, and 5 from Bins 3, 4, and 6. Comparing the results shown on Figure 6.13-26, three major groupings of brine chemistry evolution can be seen where not only the presence or absence of anhydrite but the presence or absence of glauberite is associated with the general trajectory of the pH. In general, the precipitation of glauberite is associated with waters in Bins 2, 4, and 5. Bins 3 and 6 are associated with arcanite. Bin 2 is characterized by the early precipitation of halite. In no cases do any calcium chloride, magnesium chloride or calcium-magnesium chloride minerals, such as bischofite and tachyhydrite, precipitate.

Source: Output DTN: MO0310SPAPCELA.002.

Figure 6.13-26. Variation of pH with Relative Humidity for All Six Dust Leachate Bins

6.13.3 Lookup Table Interpolation for Seepage and Deliquescence Conditions

Aside from the general modeling uncertainty discussed in Section 6.12, this section considers the interpolation requirements associated with implementing the lookup tables within the TSPA-LA. The lookup tables contain two types of parameters, independent and dependent. The independent parameters are relative humidity, temperature, and carbon dioxide fugacity. Values for these parameters are needed to determine the values of the dependent parameters, such as the pH, or the total concentration of a dissolved chemical component (chloride, for example).

The independent variables in the lookup tables (i.e., relative humidity, temperature, and CO_2 fugacity) have their own uncertainty in the TSPA-LA realizations. The uncertainties for temperature and relative humidity are defined outside the physical and chemical environment model and are not addressed here. As for CO_2 fugacity, tables are generated from the THC model

results in Section 6.7.2, and overall statistics on CO_2 fugacity are reported. When a given water type is selected for any given TSPA-LA model realization, the $p\text{CO}_2$ value becomes a discrete value over the time interval in the given lookup table designation. Therefore, the interpolation range over that given time period is established by looking at the previous time step's value and the next time step's value. This gives the total range that is associated with that period. For example, when using Table 6.7-1 for the interval from 200 to 250 years, the drift $p\text{CO}_2$ is set at 4.34×10^{-4} bar. The $p\text{CO}_2$ for that period would range between 5.28×10^{-4} (the value for the preceding period) and 3.18×10^{-4} bar (the value for the following period). This range is far smaller than the overall range that is associated with in-drift $p\text{CO}_2$, as discussed in Section 6.7.2.

The lookup tables provide direct results only for select combinations of independent variables. That is, they provide results at temperatures of 40°C , 70°C , 100°C (for both seepage and dust leachates), 120°C and 140°C for dust leachates, CO_2 fugacities of 10^{-2} , 10^{-3} , and 10^{-4} bar, and relative humidity at intervals up to 2 percent. Most humidity intervals are less than 2 percent. The TSPA-LA model is designed to interpolate and extrapolate ($p\text{CO}_2$ parameter only) dependent variable outputs for other combinations of these parameters (except for temperatures above 140°C and below 40°C , see Section 6.7.2.2). By interpolating and extrapolating, the lookup tables provide a set of smooth and continuous response surfaces. Although some error may be introduced by interpolation and extrapolation, this error is negligible compared to model uncertainty and uncertainty in the predicted values of the independent variables (see Section 6.12 for uncertainty analysis).

6.13.4 Chemical Environments on the Drip Shield and Waste Package

In addition to pH and ionic strength, the main parameter of interest for drip shield performance is the concentration of F in the solution, because fluoride has a strong influence on titanium corrosion rates. For the waste package environment, the primary aqueous components of concern include Cl, N, and S, and to some extent other halides such as Br, because high concentrations of these elements enhance corrosion of Alloy 22. In addition to these chemical parameters, other particular parameters of interest are deliquescence points, brine compositions, and brine evolution. Each of these is discussed in terms of the two major outputs of this model, the composition of in-drift seepage and dust leachate type waters.

In order to develop an argument that supports the use of probabilities and distributions for the seepage water inputs, an assumption is carried forward into this report (see Assumption 5.1.4 for basis and further discussion). That is the five THC starting waters adequately represent all possible seepage waters, and are therefore used to initiate this abstraction and their bin distributions (Table 6.6-4), as discussed in Section 6.6.

6.13.4.1 Seepage

From Tables 6.13-1 through 6.13-3, waters from Bins 1 and 2 are not deemed to be relevant for the waste package or drip shield, and there is some correlation through time for which bins are most likely. For pH, Figure 6.13-15 shows that the seepage pH range varies from bin to bin as a function of relative humidity. The overall pH range is approximately 10.5 to 4.5. For Bin 3, the range is from about 8 to 4.5. As shown on Table 6.13-1, the time-integrated percentage of all of the 368 starting waters represented by this bin is less than 1 percent. For Bins 4 and 5, the pH

range is between 6.5 and 8.5. These two bins account for about 20 percent of the locations on the bin history map (Table 6.6-4), but only have a time-integrated probability of occurrence, in the first 20,000 years, of about 1.5 percent. For the remaining 70 percent of the starting waters (Bins 6 through 11) used in the abstraction, the pH range is from about 8 to 10.5. Therefore, the most likely pH range of seepage water on the waste package is from approximately 8 to 10.5. Bins 6 through 11 also represent 98 percent of the time-integrated bin probability (for the 20,000-year regulatory time interval).

Figure 6.13-27 shows the predicted concentrations of F for the lookup tables representing Bins 3 through 11. The figure indicates that the maximum molality that could be present is about 1. This occurs at a drift relative humidity above about 90 percent. The maximum values fall within Bins 9 and 6. Bin 9 has a high probability of occurrence in the boiling, hot, and cool-down periods. Possible Cl concentrations are much higher, up to about 10 molal at low relative humidity (Figure 6.13-28), and are relatively insensitive to bin choice.

Source: Output DTN: MO0312SPAPCESA.002.

Figure 6.13-27. Range of F Versus Relative Humidity for the Seepage Evaporation Lookup Tables Representing Bins 3 through 11

Source: Output DTN: MO0312SPAPCESA.002.

Figure 6.13-28. Range of Cl Versus Relative Humidity for the Seepage Evaporation Lookup Tables Representing Bins 3 through 11

Table 6.13-8 shows the brine compositions that develop during evaporative concentration of the EBS seepage waters, as presented in the TSPA-LA lookup tables. Also shown is the endpoint relative humidity of the brines represented by the 11 bins. Under most conditions, the seepage waters can be classified as one of three brine types: sodium chloride, sodium carbonate, or calcium chloride. Bins 1 through 3 show the accumulation of Ca and Cl is sufficient to make them the dominant cation and anion, respectively, as relative humidity decreases. Under these conditions, the potential for aggressive localized corrosion exists. However, based on the bin history maps (Figure 6.13-1) bins 1 and 2 are not possible as crown seepage and the time integrated bin probability for Bin 3 over the 20,000-year regulatory timeframe is 0.22 percent (Table 6.13-1). In fact, Bin 3 waters only occur during the first several hundred years (Figure 6.13-1) when drift temperatures are high and liquid water is least likely to enter the drift. With the exception of Bins 8 through 10, the dominant anion is Cl, which could provide for corrosion potential (~72 percent), yet Bins 4 through 7 and 11 are not expected to be as aggressive as Bin 3 because of the absence of CaCl_2 . Also evident from Figure 6.13-29 is the potential for six of the bins to have a CLN ratio above 10 at relative humidity conditions above 70 percent. In Bins 6 and 7, Cl:N ratios above 30 are possible. Bin 7 is associated with the cool down and preclosure periods and has a relatively high probability of occurrence in the 10,000- to 20,000-year interval (Figure 6.13-1). Bin 6 is associated with the hotter waste package temperatures that occur early in the repository history, and waters in this bin are much less likely to occur.

Source: Output DTN: MO0312SPAPCESA.002.

Figure 6.13-29. Range of Cl to N Molal Ratios for the Seepage Evaporation Lookup Tables Representing Bins 3 through 11

Additional plots have been included in the following figures to show the ranges in Bins 3 through 11 for total Ca, S, and C (Figures 6.13-30 through 6.13-32). Plots for Si, N, K, Mg, and Na are provided in *checked MOALT R0d2.xls* archived in DTN: MO0312SPAPCESA.002.

Source: Output DTN: MO0312SPAPCESA.002.

Figure 6.13-30. Range of Total Elemental Ca for the Seepage Evaporation Lookup Tables Representing Bins 3 through 11

Source: Output DTN: MO0312SPAPCESA.002.

Figure 6.13-31. Range of Total Elemental S for the Seepage Evaporation Lookup Tables Representing Bins 3 through 11

Source: Output DTN: MO0312SPAPCESA.002.

Figure 6.13-32. Range of Total Elemental C for the Seepage Evaporation Lookup Tables Representing Bins 3 through 11

Somewhere between 100 and 95 percent relative humidity in the drift, the ionic strength of the evaporating solutions will go above 1 molal (Figure 6.13-33). At lower relative humidity conditions, concentrations of well over 10 molal are possible. EQ6 results report the relative loss of water mass through the evaporative process. Figure 6.13-34 plots this water loss against the ionic strength. This figure shows that when the brines are very concentrated, the relative mass of water becomes extremely small. For example, when 1 kg of seepage water is concentrated to ionic strengths of 10 or greater, the mass of remaining water has become a gram or less. In some cases, the remaining brine is 10^{-4} grams or less. This indicates that the overall corrosion capability of the brines reacting with the waste package or drip shield should decrease as evaporation increases due to the substantial reduction in seepage water mass.

Source: Output DTN: MO0312SPAPCESA.002.

Figure 6.13-33. Range of Ionic Strength Versus Relative Humidity for the Seepage Evaporation Lookup Tables Representing Bins 3 through 11

Source: Output DTN: MO0312SPAPCESA.002.

Figure 6.13-34. Mass of Water Versus Ionic Strength for the Seepage Evaporation Lookup Tables Representing Bins 3 through 11

The mineral assemblages associated with Bins 3 through 11 are provided on Table 6.13-6. These minerals are likely to form on drip shield and waste package surfaces as seepage evaporites.

6.13.4.2 Dust Leachate

For a given set of temperatures, $p\text{CO}_2$, and humidity values, the chemical parameters that are most relevant to waste package degradation include pH, Cl, Cl/NO₃, and (Cl + F)/(NO₃ + SO₄). From the lookup table calculations, it is determined that the brine pH is more sensitive to the in-drift temperature and $p\text{CO}_2$ changes than to the other parameters. Figure 6.13-26 shows that a decrease in $p\text{CO}_2$ from 10^{-2} to 10^{-4} bar would systematically increase pH by one unit over the whole evaporation range. To illustrate this effect, Figure 6.13-26 shows three groupings of curves for each bin. These three groupings reflect the $p\text{CO}_2$ concentrations trending downward from lowest to highest. As a result of the decrease of $p\text{CO}_2$, carbonate minerals precipitate, and the concentrations of Ca and Mg decrease. However, the effect of temperature on brine pH is more complicated and varies with humidity. Temperature effects are shown on Figure 6.13-26 by examining each bundle of five lines that is associated with a given $p\text{CO}_2$ group. A change in temperature from 40 to 140°C generally results in pH variations of less than one-half a pH unit.

Table 6.13-8. Engineered Barrier System Seepage Lookup Table End Point Relative Humidity and Brine Evolution

Lookup Table File Name	Number of Se Binning Files Matching this Sensitivity Run (number of waters in bin)	% of 368 Binning Runs	Bin	Temp.	Pco ₂	Endpoint RH	88% RH Brine	85% RH Brine	82% RH Brine	Endpoint Brine
01c211e.xls.xls	5	1.4%	1	100	1.00E-02	20.0%	Ca-O	Ca-O	Ca-O	Ca-O
01c214e.xls.xls			1	40	1.00E-02	18.1%	Ca-O	Ca-O	Ca-O	Ca-O
01c217e.xls.xls			1	70	1.00E-02	19.7%	Ca-O	Ca-O	Ca-O	Ca-O
01c219e.xls.xls			1	100	1.00E-02	20.0%	Ca-O	Ca-O	Ca-O	Ca-O
01c244e.xls.xls			1	40	1.00E-03	18.1%	Ca-O	Ca-O	Ca-O	Ca-O
01c247e.xls.xls			1	70	1.00E-03	19.7%	Ca-O	Ca-O	Ca-O	Ca-O
01c249e.xls.xls			1	100	1.00E-04	20.0%	Ca-O	Ca-O	Ca-O	Ca-O
01c241e.xls.xls			1	40	1.00E-04	18.2%	Ca-O	Ca-O	Ca-O	Ca-O
01c243e.xls.xls			1	70	1.00E-04	18.7%	Ca-O	Ca-O	Ca-O	Ca-O
01c245e.xls.xls			1	100	1.00E-05	24.0%	Na-O	Na-O	Na-O	Ca-O
02c211e.xls.xls	13	3.6%	2	100	1.00E-02	20.0%	Na-O	Na-O	Na-O	Ca-O
02c214e.xls.xls			2	40	1.00E-02	20.1%	Na-O	Na-O	Na-O	Ca-O
02c217e.xls.xls			2	70	1.00E-02	21.4%	Na-O	Na-O	Na-O	Ca-O
02c219e.xls.xls			2	100	1.00E-03	24.0%	Na-O	Na-O	Na-O	Ca-O
02c244e.xls.xls			2	40	1.00E-03	21.1%	Na-O	Na-O	Na-O	Ca-O
02c247e.xls.xls			2	70	1.00E-03	24.0%	Na-O	Na-O	Na-O	Ca-O
02c249e.xls.xls			2	100	1.00E-04	24.0%	Na-O	Na-O	Na-O	Ca-O
02c241e.xls.xls			2	40	1.00E-04	21.1%	Na-O	Na-O	Na-O	Ca-O
02c243e.xls.xls			2	70	1.00E-04	24.0%	Na-O	Na-O	Na-O	Ca-O
02c245e.xls.xls			2	100	1.00E-05	43.9%	Na-O	Na-O	Na-O	K-O
03c211e.xls.xls	12	3.3%	3	100	1.00E-02	20.0%	Na-O	Na-O	Na-O	Ca-O
03c214e.xls.xls			3	40	1.00E-02	20.0%	Na-O	Na-O	Na-O	Ca-O
03c217e.xls.xls			3	70	1.00E-02	22.3%	Na-O	Na-O	Na-O	K-O
03c219e.xls.xls			3	100	1.00E-03	44.0%	Na-O	Na-O	Na-O	K-O
03c244e.xls.xls			3	40	1.00E-03	20.0%	Na-O	Na-O	Na-O	Ca-O
03c247e.xls.xls			3	70	1.00E-03	42.5%	Na-O	Na-O	Na-O	K-O
03c249e.xls.xls			3	100	1.00E-04	47.4%	Na-O	Na-O	Na-O	K-O
03c241e.xls.xls			3	40	1.00E-04	20.0%	Na-O	Na-O	Na-O	Na-N
03c243e.xls.xls			3	70	1.00E-04	22.3%	Na-O	Na-O	Na-N	Na-N
03c245e.xls.xls			3	100	1.00E-05	47.4%	Na-O	Na-O	K-O	K-O
04c211e.xls.xls	43	11.7%	4	100	1.00E-02	47.4%	Na-O	Na-O	Na-N	Na-N
04c214e.xls.xls			4	40	1.00E-02	20.0%	Na-O	Na-O	Na-N	Na-N
04c217e.xls.xls			4	70	1.00E-02	22.3%	Na-O	Na-O	Na-N	Na-N
04c219e.xls.xls			4	100	1.00E-03	47.4%	Na-O	Na-O	K-O	K-O
04c244e.xls.xls			4	40	1.00E-03	20.0%	Na-O	Na-O	Na-N	Na-N
04c247e.xls.xls			4	70	1.00E-03	22.3%	Na-O	Na-O	Na-N	Na-N
04c249e.xls.xls			4	100	1.00E-04	80.0%	Na-O	Na-O	Na-N	Na-N
04c241e.xls.xls			4	40	1.00E-04	20.0%	Na-O	Na-O	Na-N	Na-N
04c243e.xls.xls			4	70	1.00E-04	22.3%	Na-O	Na-O	Na-N	Na-N
04c245e.xls.xls			4	100	1.00E-05	80.1%	Na-O	Na-O	Na-N	Na-N
05c211e.xls.xls	27	7.3%	5	100	1.00E-02	80.1%	Na-O	Na-O	No Brine	Na-O
05c214e.xls.xls			5	40	1.00E-02	20.0%	Na-O	Na-O	No Brine	Na-O
05c217e.xls.xls			5	70	1.00E-02	22.3%	Na-O	Na-O	No Brine	K-O
05c219e.xls.xls			5	100	1.00E-03	80.1%	Na-O	Na-O	No Brine	Na-O
05c244e.xls.xls			5	40	1.00E-03	20.0%	Na-O	Na-O	No Brine	Na-O
05c247e.xls.xls			5	70	1.00E-03	22.3%	Na-O	Na-O	No Brine	K-O
05c249e.xls.xls			5	100	1.00E-04	80.1%	Na-O	Na-O	No Brine	Na-O
05c241e.xls.xls			5	40	1.00E-04	20.0%	Na-O	Na-O	No Brine	Na-N
05c243e.xls.xls			5	70	1.00E-04	22.3%	Na-O	Na-O	No Brine	K-O
05c245e.xls.xls			5	100	1.00E-05	80.1%	Na-O	Na-O	No Brine	Na-O
06c211e.xls.xls	8	2.2%	6	100	1.00E-02	80.1%	Na-O	Na-O	No Brine	Na-O
06c214e.xls.xls			6	40	1.00E-02	20.0%	Na-O	Na-O	No Brine	Na-N
06c217e.xls.xls			6	70	1.00E-02	22.3%	Na-O	Na-O	No Brine	K-O
06c219e.xls.xls			6	100	1.00E-03	80.1%	Na-O	Na-O	No Brine	Na-O
06c244e.xls.xls			6	40	1.00E-03	20.0%	Na-O	Na-O	No Brine	Na-N
06c247e.xls.xls			6	70	1.00E-03	22.3%	Na-O	Na-O	No Brine	K-O
06c249e.xls.xls			6	100	1.00E-04	80.1%	Na-O	Na-O	No Brine	Na-O
06c241e.xls.xls			6	40	1.00E-04	20.0%	Na-O	Na-O	No Brine	Na-N
06c243e.xls.xls			6	70	1.00E-04	22.3%	Na-O	Na-O	No Brine	K-O
06c245e.xls.xls			6	100	1.00E-05	80.1%	Na-O	Na-O	No Brine	Na-O

Table 6.13-8. Engineered Barrier System Seepage Lookup Table End Point Relative Humidity and Brine Evolution (Continued)

07c211a.xls.xls	35	6.6%	7	100	1.00E-02	59.1%	Na-C	Na-C	Na-C	K-Cl
07c219a.xls.xls			7	40	1.00E-02	63.0%	Na-C	Na-C	Na-C	Na-H
07c217a.xls.xls			7	70	1.00E-02	60.5%	Na-C	Na-C	Na-C	K-Cl
07c215a.xls.xls			7	100	1.00E-02	59.1%	Na-C	Na-C	Na-C	Na-C
07c214a.xls.xls			7	40	1.00E-02	61.7%	Na-C	Na-C	Na-C	Na-H
07c212a.xls.xls			7	70	1.00E-02	59.7%	Na-C	Na-C	Na-C	K-Cl
07c411a.xls.xls			7	100	1.00E-04	60.0%	Na-C	Na-C	Na-C	Na-C
07c409a.xls.xls			7	40	1.00E-04	66.2%	Na-C	Na-C	No Brine	Na-C
07c417a.xls.xls			7	70	1.00E-04	59.8%	Na-C	Na-C	Na-C	K-Cl
08c211a.xls.xls			8	100	1.00E-02	59.1%	Na-C	Na-C	Na-C	K-Cl
08c219a.xls.xls	22	6.0%	8	40	1.00E-02	63.0%	Na-C	Na-C	Na-H	Na-H
08c217a.xls.xls			8	70	1.00E-02	60.5%	Na-C	Na-C	Na-C	K-Cl
08c215a.xls.xls			8	100	1.00E-02	59.1%	Na-C	Na-C	Na-C	Na-C
08c214a.xls.xls			8	40	1.00E-02	61.7%	Na-C	Na-C	Na-C	Na-H
08c212a.xls.xls			8	70	1.00E-02	59.7%	Na-C	Na-C	Na-C	K-Cl
08c411a.xls.xls			8	100	1.00E-04	59.9%	Na-C	Na-C	Na-C	Na-C
08c409a.xls.xls			8	40	1.00E-04	62.2%	Na-C	Na-C	Na-C	Na-C
08c417a.xls.xls			8	70	1.00E-04	59.8%	Na-C	Na-C	Na-C	K-Cl
09c211a.xls.xls			9	100	1.00E-02	59.8%	Na-C	Na-C	Na-C	K-Cl
09c219a.xls.xls			9	40	1.00E-02	63.0%	Na-C	Na-C	Na-C	K-N
09c217a.xls.xls	58	15.8%	9	70	1.00E-02	59.0%	Na-C	Na-C	Na-C	K-N
09c215a.xls.xls			9	100	1.00E-02	59.9%	Na-C	Na-C	Na-C	K-Cl
09c214a.xls.xls			9	40	1.00E-02	61.3%	Na-C	Na-C	Na-C	K-N
09c212a.xls.xls			9	70	1.00E-02	57.5%	Na-C	Na-C	Na-C	K-N
09c411a.xls.xls			9	100	1.00E-04	62.3%	Na-C	Na-C	Na-C	K-N
09c409a.xls.xls			9	40	1.00E-04	62.1%	Na-C	Na-C	Na-C	K-N
09c417a.xls.xls			9	70	1.00E-04	49.8%	Na-C	Na-C	Na-C	K-N
10c211a.xls.xls			10	100	1.00E-02	59.0%	Na-C	Na-C	Na-C	Na-C
10c219a.xls.xls			10	40	1.00E-02	66.1%	Na-C	Na-C	No Brine	Na-C
10c217a.xls.xls			10	70	1.00E-02	60.3%	Na-C	Na-C	Na-C	K-Cl
10c215a.xls.xls	10	2.7%	10	100	1.00E-02	59.0%	Na-C	Na-C	Na-C	Na-C
10c214a.xls.xls			10	40	1.00E-02	61.5%	Na-C	Na-C	Na-C	Na-H
10c212a.xls.xls			10	70	1.00E-02	59.6%	Na-C	Na-C	Na-C	K-Cl
10c411a.xls.xls			10	100	1.00E-04	58.8%	Na-C	Na-C	Na-C	Na-C
10c409a.xls.xls			10	40	1.00E-04	62.1%	Na-C	Na-C	Na-C	Na-H
10c417a.xls.xls			10	70	1.00E-04	59.5%	Na-C	Na-C	Na-C	K-Cl
11c211a.xls.xls			11	100	1.00E-02	59.0%	Na-C	Na-C	Na-C	Na-C
11c219a.xls.xls			11	40	1.00E-02	62.7%	Na-C	Na-C	Na-C	Na-H
11c217a.xls.xls			11	70	1.00E-02	60.4%	Na-C	Na-C	Na-C	K-Cl
11c215a.xls.xls			11	100	1.00E-02	59.0%	Na-C	Na-C	Na-C	Na-C
11c214a.xls.xls	145	39.4%	11	40	1.00E-02	61.5%	Na-C	Na-C	Na-C	Na-H
11c212a.xls.xls			11	70	1.00E-02	59.6%	Na-C	Na-C	Na-C	K-Cl
11c411a.xls.xls			11	100	1.00E-04	58.8%	Na-C	Na-C	Na-C	Na-C
11c409a.xls.xls			11	40	1.00E-04	62.1%	Na-C	Na-C	Na-C	Na-H
11c417a.xls.xls			11	70	1.00E-04	59.5%	Na-C	Na-C	Na-C	K-Cl
11c415a.xls.xls			11	100	1.00E-04	58.8%	Na-C	Na-C	Na-C	Na-C
11c413a.xls.xls			11	40	1.00E-04	62.1%	Na-C	Na-C	Na-C	Na-H
11c411a.xls.xls			11	70	1.00E-04	59.5%	Na-C	Na-C	Na-C	K-Cl
11c409a.xls.xls			11	100	1.00E-04	58.8%	Na-C	Na-C	Na-C	Na-C
11c407a.xls.xls			11	40	1.00E-04	59.5%	Na-C	Na-C	Na-C	K-Cl

Source: Output DTN: MO0312SPAPCESA.002.

NOTE: Shown on the table is the percentage of all waters the bins represent. To see the time normalized percentages for the crown and invert, see Tables 6.13-1 and 6.13-2.

The variations of brine chemistry among the six representative dusts are shown in Figure 6.13-26 and Figures 6.13-35 through 6.13-40. Figure 6.13-26 indicates that the maximum pH that can occur in deliquescent water on the waste packages is 11.7, ranging down to a value slightly greater than 6. Figure 6.13-35 shows that F concentrations are less than one molal for all samples during evaporation because of the precipitation of CaF_2 . Figure 6.13-36 indicates that the ionic strength ranges from 10^{-3} molal to values as great as ~50 molal at low humidities. Figure 6.13-37 shows at low humidity, the brine condensed on dust could have Cl concentrations as high as 9 molal. The NO_3 concentrations can be as high as ~20 molal (Figure 6.13-39). Figure 6.13-24 and 6.13-38 show that high ratios of Cl/NO_3 and $(\text{Cl} + \text{F})/(\text{NO}_3 + \text{SO}_4)$ occur only for dust leachate Bin 6, at relative humidity values greater than 50 percent. At least 81 percent of waste packages will never be exposed to deliquescent brine with a Cl/NO_3 ratio higher than one (Figure 6.13-38 and Table 6.13-9). This value does not account for uncertainty. The difference between Figure 6.13-24 and Figure 6.13-38 is mainly due to SO_4 concentrations, which could be as high as 2 molal.

Source: Output DTN: MO0310SPAPCELA.002.

Figure 6.13-35. Variation of F Concentration with Relative Humidity for All Six Dust Leachate Bins

Source: Output DTN: MO0310SPAPCELA.002.

Figure 6.13-36. Variation of Ionic Strength with Relative Humidity for All Six Dust Leachate Bins

Source: Output DTN: MO0310SPAPCELA.002.

Figure 6.13-37. Variation of Cl Concentration with Relative Humidity for All Six Dust Leachate Bins

Source: Output DTN: MO0310SPAPCELA.002.

Figure 6.13-38. Variation of Cl/NO₃ with Relative Humidity for All Six Dust Leachate Bins

Source: Output DTN: MO0310SPAPCELA.002.

Figure 6.13-39. Variation of NO_3 with Relative Humidity for All Six Dust Leachate Bins

Figure 6.12-5 shows the concentrations of Br that can occur in brines formed by dust deliquescence. These values can get as high as ~6 molal. Although the presence of relatively high Br concentrations could be an artifact of the bromide in the dusts being derived from LiBr-containing construction water (Peterman et al. 2003 [DIRS 162819]), the fact that high Br concentrations can occur in the seepage water (Figure 6.12.4-1) indicates that this may be a real effect. Section 6.12.4.2.4 discusses on the uncertainty associated with Br in dust samples.

Figure 6.13-40 shows how the mass of solvent and ionic strength vary with relative humidity. The mass of solvent becomes less than 10^{-4} kg $\text{H}_2\text{O}/20$ grams of dust before the evaporation reaches the minimum deliquescence point. At such low water/solid ratios, there is sufficient liquid water to only form a few molecular layers on the dust surface. This very small amount of water is insufficient to form a continuous water film on waste packages.

Source: Output DTN: MO0310SPAPCELA.002.

Figure 6.13-40. Mass of Water Versus Ionic Strength for All 6 Dust Leachate Bins

Additional plots can be found for aqueous concentrations of C, S, and Ca in *newDustMOALT.xls* archived in DTN: MO0310SPAPCELA.002.

Table 6.13-9 shows the brine compositions that develop by evaporative concentration of the dust leachate, using the data in the dust leachate lookup tables. Also shown in this figure is the endpoint relative humidity of the brines represented by the six dust leachate bin waters. Under most conditions, the dust leachate waters tend to be classified as sodium nitrate, sodium sulfate, potassium nitrate, sodium chloride, or calcium nitrate brines. Only Bin 1 shows sufficient accumulation of Ca to make it the dominant cation, yet the dominant anion in this bin at all relative humidities is nitrate, which inhibits corrosion. Bins 3 and 6 are the only bins that show any generation of a chloride-type brine. Based on the given distribution, this could occur about 19.2 percent of the time (Table 6.13-9). However, the N concentration in these waters is fairly high and could inhibit potential for localized corrosion (BSC 2004 [DIRS 169984], Section 6.4.4.3.2). Bin 3 and 6 waters also have the highest pH values. In the most likely case (Bin 5), the evolution of the brine is from a sodium nitrate water to a potassium nitrate or a sodium bromide type water.

Table 6.13-7 contains the mineral assemblages that are likely to comprise the soluble dust mineral phases sitting on the waste packages and drip shield.

6.13.5 The Chemical Environment in the Invert

The chemical environment in the invert is important for two key TSPA-LA parameters, radionuclide solubility and colloid stability. In general, the chemical parameters of interest are

pH and ionic strength. All 11 sets of bin chemistries are possible in the invert, whereas the drip shield and waste package environment discussed in Section 6.13.4 did not consider Bins 1 and 2, as they do not occur in the crown seepage waters. To establish the chemical environment in the invert, multiple sources of water must be considered. These include waters that have wicked into the invert from below, dripped from the crown, drip shield, or outer surface of the waste package, or exited from a breached waste package after interacting with the waste form.

Table 6.13-9. Dust Leachate Lookup Table End Point Relative Humidity and Brine Evolution

Lookup Table File Name	Number of 60 Binning Files Matching this Sensitivity Run	% of 62 Binning Output Runs	Bin	Temp.	P_{CO_2}	Endpoint RH	95% RH Brine	85% RH Brine	65% RH Brine	Endpoint Brine
d1c204.xls	3	5.8	1	40	1.00E-02	50.0%	Na-N	Na-N	Na-N	Ca-N
d1c207.xls			1	70	1.00E-02	30.0%	Na-N	Na-N	Na-N	Ca-N
d1c210.xls			1	100	1.00E-02	31.5%	Na-N	Na-N	Na-N	Ca-N
d1c212.xls			1	120	1.00E-02	30.8%	Na-N	Na-N	Na-N	Ca-N
d1c214.xls			1	140	1.00E-02	26.2%	Na-N	Na-N	Na-N	Na-N
d1c304.xls			1	40	1.00E-03	50.0%	Na-N	Na-N	Na-N	Ca-N
d1c307.xls			1	70	1.00E-03	30.0%	Na-N	Na-N	Na-N	Ca-N
d1c310.xls			1	100	1.00E-03	31.5%	Na-N	Na-N	Na-N	Ca-N
d1c312.xls			1	120	1.00E-03	30.7%	Na-N	Na-N	Na-N	Ca-N
d1c314.xls			1	140	1.00E-03	26.2%	Na-N	Na-N	Na-N	Na-N
d1c404.xls			1	40	1.00E-04	50.0%	Na-N	Na-N	Na-N	Ca-N
d1c407.xls			1	70	1.00E-04	30.0%	Na-N	Na-N	Na-N	Ca-N
d1c410.xls			1	100	1.00E-04	32.4%	Na-N	Na-N	Na-N	Ca-N
d1c412.xls			1	120	1.00E-04	30.8%	Na-N	Na-N	Na-N	Ca-N
d1c414.xls			1	140	1.00E-04	26.2%	Na-N	Na-N	Na-N	Na-N
d2c204.xls	4	7.7	2	40	1.00E-02	58.1%	Na-N	Na-N	Na-N	Na-N
d2c207.xls			2	70	1.00E-02	47.8%	Na-N	Na-N	Na-N	Na-N
d2c210.xls			2	100	1.00E-02	42.2%	Na-N	Na-N	Ca-N	Ca-N
d2c212.xls			2	120	1.00E-02	35.4%	Na-N	Na-N	Ca-N	Ca-N
d2c214.xls			2	140	1.00E-02	32.0%	Na-N	Na-N	Ca-N	Ca-N
d2c304.xls			2	40	1.00E-03	58.1%	Na-N	Na-N	Na-N	Na-N
d2c307.xls			2	70	1.00E-03	47.8%	Na-N	Na-N	Na-N	Na-N
d2c310.xls			2	100	1.00E-03	42.2%	Na-N	Na-N	Ca-N	Ca-N
d2c312.xls			2	120	1.00E-03	35.4%	Na-N	Na-N	Ca-N	Ca-N
d2c314.xls			2	140	1.00E-03	32.0%	Na-N	Na-N	Ca-N	Ca-N
d2c404.xls			2	40	1.00E-04	58.1%	Na-N	Na-N	Na-N	Na-N
d2c407.xls			2	70	1.00E-04	47.8%	Na-N	Na-N	Na-N	Ca-N
d2c410.xls			2	100	1.00E-04	42.2%	Na-N	Na-N	Ca-N	Ca-N
d2c412.xls			2	120	1.00E-04	35.4%	Na-N	Na-N	Ca-N	Ca-N
d2c414.xls			2	140	1.00E-04	32.0%	Na-N	Na-N	Ca-N	Ca-N
d3c204.xls	9	17.3	3	40	1.00E-02	60.6%	Na-S	Na-CI	Na-CI	Na-N
d3c207.xls			3	70	1.00E-02	49.9%	Na-S	Na-S	Na-CI	Ca-N
d3c210.xls			3	100	1.00E-02	42.8%	Na-S	Na-S	Na-CI	Ca-N
d3c212.xls			3	120	1.00E-02	36.4%	Na-S	Na-S	Na-CI	Ca-N
d3c214.xls			3	140	1.00E-02	32.4%	Na-S	Na-S	Na-CI	Ca-N
d3c304.xls			3	40	1.00E-03	58.8%	Na-S	Na-S	Na-CI	Na-N
d3c307.xls			3	70	1.00E-03	50.0%	Na-S	Na-S	Na-CI	Na-N
d3c310.xls			3	100	1.00E-03	43.2%	Na-S	Na-S	Na-CI	Ca-N
d3c312.xls			3	120	1.00E-03	38.0%	Na-S	Na-S	Na-CI	Ca-N
d3c314.xls			3	140	1.00E-03	32.6%	Na-S	Na-S	Na-CI	Ca-N
d3c404.xls			3	40	1.00E-04	58.8%	Na-S	Na-S	Na-CI	Na-N
d3c407.xls			3	70	1.00E-04	50.0%	Na-S	Na-S	Na-CI	Na-N
d3c410.xls			3	100	1.00E-04	43.4%	Na-S	Na-S	Na-CI	Ca-N
d3c412.xls			3	120	1.00E-04	38.6%	Na-S	Na-S	Na-CI	Ca-N
d3c414.xls			3	140	1.00E-04	32.6%	Na-S	Na-S	Na-CI	Ca-N

Table 6.13-9. Dust Leachate Lookup Table End Point Relative Humidity and Brine Evolution (Continued)

d4c2104.xls	12	23.1	4	40	1.00E-02	52.9%	Na-N	Na-N	Na-N	Na-Br
d4c2107.xls			4	70	1.00E-02	45.4%	Na-N	Na-N	Na-N	Na-N
d4c2110.xls			4	100	1.00E-02	36.4%	Na-N	Na-N	Na-N	Na-N
d4c2112.xls			4	120	1.00E-02	31.2%	Na-N	Na-N	Na-N	Na-N
d4c2114.xls			4	140	1.00E-02	26.4%	Na-N	Na-N	Na-N	Na-N
d4c2116.xls			4	40	1.00E-03	52.9%	Na-N	Na-N	Na-N	Na-Br
d4c2107.xls			4	70	1.00E-03	44.5%	Na-N	Na-N	Na-N	Na-N
d4c2110.xls			4	100	1.00E-03	36.4%	Na-N	Na-N	Na-N	Na-N
d4c2112.xls			4	120	1.00E-03	31.2%	Na-N	Na-N	Na-N	Na-N
d4c2114.xls			4	140	1.00E-03	26.4%	Na-N	Na-N	Na-N	Na-N
d4c4104.xls			4	40	1.00E-04	52.9%	Na-N	Na-N	Na-N	Na-Br
d4c4107.xls			4	70	1.00E-04	44.5%	Na-N	Na-N	Na-N	Na-N
d4c4110.xls			4	100	1.00E-04	36.4%	Na-N	Na-N	Na-N	Na-N
d4c4112.xls			4	120	1.00E-04	31.2%	Na-N	Na-N	Na-N	Na-N
d4c4114.xls			4	140	1.00E-04	26.4%	Na-N	Na-N	Na-N	Na-N
d5c2104.xls	23	44.2	5	40	1.00E-02	56.1%	Na-N	Na-N	Na-N	Na-Br
d5c2107.xls			5	70	1.00E-02	45.2%	Na-N	Na-N	Na-N	Na-N
d5c2110.xls			5	100	1.00E-02	41.8%	Na-N	Na-N	Na-N	K-N
d5c2112.xls			5	120	1.00E-02	31.1%	Na-N	Na-N	Na-N	Na-N
d5c2114.xls			5	140	1.00E-02	26.3%	Na-N	Na-N	Na-N	Na-N
d5c3104.xls			5	40	1.00E-03	56.1%	Na-N	Na-N	Na-N	Na-Br
d5c3107.xls			5	70	1.00E-03	45.2%	Na-N	Na-N	Na-N	Na-N
d5c3110.xls			5	100	1.00E-03	41.8%	Na-N	Na-N	Na-N	K-N
d5c3112.xls			5	120	1.00E-03	31.1%	Na-N	Na-N	Na-N	Na-N
d5c3114.xls			5	140	1.00E-03	26.3%	Na-N	Na-N	Na-N	Na-N
d5c4104.xls			5	40	1.00E-04	56.1%	Na-N	Na-N	Na-N	Na-Br
d5c4107.xls			5	70	1.00E-04	45.2%	Na-N	Na-N	Na-N	Na-N
d5c4110.xls			5	100	1.00E-04	41.8%	Na-N	Na-N	Na-N	K-N
d5c4112.xls			5	120	1.00E-04	31.1%	Na-N	Na-N	Na-N	Na-N
d5c4114.xls			5	140	1.00E-04	26.3%	Na-N	Na-N	Na-N	Na-N
d6c2104.xls	1	1.9	6	40	1.00E-02	59.8%	Na-C	Na-C	Na-C	Na-Br
d6c2107.xls			6	70	1.00E-02	55.9%	Na-C	Na-C	Na-C	K-N
d6c2110.xls			6	100	1.00E-02	42.8%	Na-C	Na-C	Na-C	K-N
d6c2112.xls			6	120	1.00E-02	36.4%	Na-C	Na-C	Na-C	K-N
d6c2114.xls			6	140	1.00E-02	32.3%	Na-C	Na-C	Na-C	K-N
d6c3104.xls			6	40	1.00E-03	59.4%	Na-C	Na-C	Na-C	Na-Cl
d6c3107.xls			6	70	1.00E-03	49.7%	Na-C	Na-C	Na-C	K-N
d6c3110.xls			6	100	1.00E-03	43.2%	Na-C	Na-C	Na-C	K-N
d6c3112.xls			6	120	1.00E-03	38.5%	Na-C	Na-C	Na-C	K-N
d6c3114.xls			6	140	1.00E-03	32.6%	Na-C	Na-C	Na-C	K-N
d6c4104.xls			6	40	1.00E-04	58.3%	Na-C	Na-C	Na-C	Na-Cl
d6c4107.xls			6	70	1.00E-04	49.4%	Na-C	Na-C	Na-C	K-N
d6c4110.xls			6	100	1.00E-04	43.4%	Na-C	Na-C	Na-C	K-N
d6c4112.xls			6	120	1.00E-04	38.6%	Na-C	Na-C	Na-C	K-N
d6c4114.xls			6	140	1.00E-04	32.7%	Na-C	Na-C	Na-C	K-N

Source: Output DTN: MO0310SPAPCELA.002.

Figure 6.13-1 shows the bin history maps for each of the five waters in a color-coded scheme. This figure illustrates that the waters being wicked into the invert are chemically distinct from the waters seeping from the crown over significant portions during the early periods (i.e., the boiling and hot periods; Table 6.13-3). In addition, the temperature, $p\text{CO}_2$, and relative humidity will not be the same in the drift as in the invert throughout time (Section 6.7.2). This indicates that, even though the waters wicking into the invert and seeping into the invert from the crown of the drift come from the same bin, the chemistry parameters that are obtained from a given lookup table could be different. During certain time periods there is also the possibility that seepage that has entered the waste package, and become chemically modified due to reactions with the waste form and in-package components, can leave the waste package and introduce yet a third type of water into the invert. Figure 6.13-41 shows the potential sources of water that can enter the invert. These three sources of water are discussed independently in the following paragraphs.

Figure 6.13-41. Schematic Representation of the Sources of Different Chemical Fluxes Into the Invert and Subsequent Radionuclide Release from the Engineered Barrier System

6.13.5.1 Crown Seepage Chemistry

Seepage chemistry is previously discussed in detail in Section 6.13.4. That section provides a description of the ranges of crown seepage waters that could enter the invert.

6.13.5.2 Invert Wicking Chemistry

In addition to the range of possible water chemistries available from crown seepage (Bins 3 through 11), waters entering the invert by wicking waters include Bins 1 and 2, as shown on Figure 6.13-1. Although the potentially corrosive waters in Bins 1 and 2 are rare over the long term (thousands of years), they are common in the invert during the boiling period, as shown on Table 6.13-3. Figure 6.13-16 and Figures 6.13-42 through 6.13-47 show the compositional (pH,

F, Cl, Ca, S, C, and ionic strength) evolution of Bin 1 and 2 waters that occurs during evaporation. Plots for Si, N, K, Mg, Na, and Cl:N ratio are not shown here, but are provided in *checked MOALT R02d2.xls* archived in DTN: MO0312SPAPCESA.002.

Source: Output DTN MO0312SPAPCESA.002.

Figure 6.13-42. Range of F Versus Relative Humidity for the Seepage Evaporation Lookup Tables Representing Bins 1 and 2

Source: Output DTN MO0312SPAPCESA.002.

Figure 6.13-43. Range of CI Versus Relative Humidity for the Seepage Evaporation Lookup Tables Representing Bins 1 and 2

Source: Output DTN MO0312SPAPCESA.002.

Figure 6.13-44. Range of Ionic Strength Versus Mass of Water (kg) for the Seepage Evaporation Lookup Tables Representing Bins 1 and 2

Source: Output DTN MO0312SPAPCESA.002.

Figure 6.13-45. Range of Total Elemental Ca for the Seepage Evaporation Lookup Tables Representing Bins 1 and 2

Source: Output DTN MO0312SPAPCESA.002.

Figure 6.13-46. Range of Total Elemental S for the Seepage Evaporation Lookup Tables Representing Bins 1 and 2

Source: Output DTN MO0312SPAPCESA.002.

Figure 6.13-47. Range of Total Elemental C for the Seepage Evaporation Lookup Tables Representing Bins 1 and 2

In contrast to crown seepage, during the boiling period the overall pH range of the waters in the invert increases, extending from ~ 8.5 down to 3.5 (Figure 6.13-16). The total range in ionic strength during this time interval, however, is similar for both crown seepage and invert wicking waters. In the hot period, Bin 4 and 5 waters are more dominant in the invert than in the crown waters and the predicted pH range extends from 6 to 10.5, as opposed to approximately 8 to 10.5 for the crown waters. For all other periods, the ranges in pH and ionic strength in the invert waters are similar to those reported for the crown seepage waters in Section 6.13.4 (pH approximately 8 to 10.5). The differences in water chemistry between the crown of the drift and the base of the invert during the boiling and hot periods are due to the temperature difference at these two localities.

6.13.5.3 Chemistry of Waste Package Leakage

The compositions of water produced in the waste package by interactions of seepage or condensate water with waste package materials and waste is documented in another process model report. That report, *In-Package Chemistry Abstraction* (BSC 2004 [DIRS 167621]), provides data containing the parameters of interest. A review of Sections 6 and 8 of *In-Package Chemistry Abstraction* (BSC 2004 [DIRS 167621]) indicates that pH and ionic strengths through time are generally much different than those reported for the crown seepage and invert wicking chemistries.

6.13.6 Comparison to Corrosion Testing Chemistries

Initial corrosion testing environments can be related to three types of natural brines: calcium chloride, carbonate, and sulfate. Initial corrosion test studies focused on the carbonate type brine,

based on reasoning that sodium carbonate type waters, as typified by J-13 well water from the saturated zone near Yucca Mountain, were the expected types of waters at the repository (Harrar et al. 1990 [DIRS 100814]). A later study (Rosenberg et al. 2001 [DIRS 154862]) showed that evaporative concentration of a water based on a reported analysis (Sonnenthal et al. 1998 [DIRS 118845]) of a porewater from Yucca Mountain resulted in a calcium chloride type brine. The types of aqueous solutions used for corrosion testing will be discussed in the context of the natural brines that follows.

Geochemical literature (e.g., Drever 1997 [DIRS 147480]) establishes the three types of brines that result from the evaporative concentration of dilute natural waters at the earth's surface: (1) calcium chloride brine, (2) carbonate brine, and (3) sulfate brine. It is important to note that the compositions of brines are dependent on relative humidity, and the dominant ions in solution can and do change as a function of relative humidity.

6.13.6.1 Corrosion Test Chemistries

Table 6.13-10 shows the composition of some of the solutions used for corrosion testing. These solutions were developed based on the evaporative concentration of a carbonate-based water with a composition based on J-13 well water, which is a saturated zone water near Yucca Mountain. The solutions represent various stages of evaporative concentration of this type of water. These aqueous solution compositions were concentrated to about 10 times (for SDW) to over 45,000 times (for SSW and BSW) to simulate evaporative concentration of the water upon contacting the waste package or the drip shield. NaCl test solutions were also used where NaCl concentrations varied from 0.5 to 4.0 molar; CaCl_2 and $\text{CaCl}_2 + \text{Ca}(\text{NO}_3)_2$ test solutions were also used with CaCl_2 concentrations up to 9 molar.

In all cases, the NO_3^- component is the most soluble species and would dominate the solution composition at the deliquescent relative humidity or eutectic point of a mineral assemblage at elevated temperatures. It is not until the relative humidity is higher that Cl^- could become comparable to NO_3^- . This is discussed in more detail in Section 6.11.2, where it is related to the transport separation of halite.

Table 6.13-10. Target Composition of Standard Test Media Based on Evaporative Concentration of a Dilute Carbonate Type Water.

Ion	SDW (mg/L)	SCW (mg/L)	SAW (mg/L)	SSW (mg/L)	BSW-12 (mg/L)
K ⁺	3.4×10^1	3.4×10^3	3.4×10^3	1.42×10^5	6.762×10^4
Na ⁺	4.09×10^2	4.09×10^4	3.769×10^4	4.87×10^4	1.0584×10^5
Mg ²⁺	1	<1	1.00×10^3	0	0
Ca ²⁺	5×10^{-1}	<1	1.00×10^3	0	0
F ⁻	1.4×10^1	1.4×10^3	0	0	1.47×10^3
Cl ⁻	6.7×10^1	6.7×10^3	2.425×10^4	1.28×10^5	1.3083×10^5
NO ₃ ⁻	6.4×10^1	6.4×10^3	2.30×10^4	1.313×10^6	1.3965×10^6
SO ₄ ²⁻	1.67×10^2	1.67×10^4	3.86×10^4	0	1.47×10^4
HCO ₃ ⁻	9.47×10^2	7.0×10^4	0	0	0
Si	27 (60°C), 49 (90°C)	27 (60°C), 49 (90°C)	27 (60°C), 49 (90°C)	0	0
pH	9.8 to 10.2	9.8 to 10.2	2.7	5.5 to 7	12

Source: DTN: LL000320405924.146 [DIRS 148327].

NOTE: The basis for the dilute carbonate water was J-13 well water, a saturated zone water near Yucca Mountain. The SDW, SCW, and BSW test solutions correspond to increasing evaporative concentration of the basis water. The SSW test solution contains only Cl⁻ and NO₃⁻ and corresponds to the scenario where the other anions have precipitated out of solution, that is, a very low relative humidity condition. The SAW test solution is a moderately acidic solution (hence no carbonate because of its volatility) with an ionic strength similar to the SCW test solution. The SAW test solution also does not contain fluoride that was excluded because of its high vapor pressure at the solution pH. pH is measured for actual solutions at room temperature.

6.13.6.2 In-Drift Brine Compared to Test Solutions

The compositions of seepage waters and waters due to deposited salt deliquescence were discussed in Sections 6.13.1 through 6.13.4. The following discussion relates those water brine types to the corrosion test solutions.

Table 6.13-11 summarizes the range of environments projected to form within the repository due to water seepage. The conditional probability (if seepage occurs at the drift crown for any particular location) that a water in a particular bin will form is also listed. For each bin, the associated brine and test solution in which corrosion testing was conducted are listed. In terms of brine type the drift crown brines are predominantly the alkaline carbonate brines, although carbonate may not be a dominant component except at higher relative humidities. The composition of each bin water as a function of temperature and relative humidity is given in lookup tables discussed in Section 6.13.1.

Table 6.13-11. Drift Crown Seepage Water and the Corresponding Corrosion Test Solutions

Bin Water	Probability of Crown Seepage ^a	Dominant Constituents in Bin Water at 98% Relative Humidity ^b	Dominant Constituents in Endpoint Brines ^b	Brine Type	Corresponding Corrosion Test Solution
1	0.00	Ca-Cl	Ca-Cl	Calcium chloride	CaCl ₂ ; CaCl ₂ + Ca(NO ₃) ₂
2	0.00	Na-Cl	Ca-Cl	Calcium chloride	CaCl ₂ ; CaCl ₂ + Ca(NO ₃) ₂
3	0.22	Na-Cl	Ca-Cl; K-Cl	Calcium chloride	CaCl ₂ ; CaCl ₂ + Ca(NO ₃) ₂
4	1.42	Na-Cl	K-NO ₃ ; Na-NO ₃	Sulfate	SSW, SAW, NaCl
5	0.79	Na-Cl	Na-Cl; K-Cl	Sulfate	SSW, SAW, NaCl
6	5.46	Na-Cl	Na-Cl; Na-NO ₃ ; K-Cl	Carbonate	SDW, SCW, BSW, SSW, NaCl
7	27.15	Na-Cl	Na-Cl; Na-NO ₃ ; K-Cl	Carbonate	SDW, SCW, BSW, SSW, NaCl
8	16.2	Na-CO ₃	Na-Cl; Na-NO ₃ ; K-Cl	Carbonate	SDW, SCW, BSW, SSW, NaCl
9	15.55	Na-CO ₃	K-NO ₃ ; K-Cl	Carbonate	SDW, SCW, BSW, SSW, NaCl
10	11.7	Na-CO ₃	Na-Cl; Na-NO ₃ ; K-Cl	Carbonate	SDW, SCW, BSW, SSW, NaCl
11	21.5	Na-Cl	Na-Cl; Na-NO ₃ ; K-Cl	Carbonate	SDW, SCW, BSW, SSW, NaCl

Source: ^a Table 6.13-1.^b Table 6.13-8.

NOTE: The probability of crown seepage represents the 20,000-year time-integrated occurrence fraction (in percent) of the representative water for each bin.

Deliquescence of dust deposited on the waste packages and drip shields is another means by which brines can form on these engineered barrier system components. The approaches used to determine the characteristics of such brines were discussed in Section 6.13.2.

Table 6.13-12 lists the brines that would develop on the waste packages using the representation of dust deliquescence developed for TSPA-LA (Sections 6.10 and 6.13.4). Included in the table are the associated brine type and the corresponding aqueous corrosion test solutions.

Table 6.13-12. Brines from Dust Deposited on the Waste Packages and the Corresponding Corrosion Test Solutions

Bin Water	Probability of Deliquescence Bin ^a	Dominant Constituents in Bin Water at 98% Relative Humidity ^b	Dominant Constituents in Endpoint Brines ^b	Brine Type	Corrosion Test Solution
1	5.77	Na-NO ₃	Ca-NO ₃	Calcium Chloride	CaCl ₂ ; CaCl ₂ + Ca(NO ₃) ₂
2	7.69	Na-NO ₃	K-NO ₃ ; Na-NO ₃	Sulfate	SSW, SAW, NaCl
3	17.31	Na-SO ₄	K-NO ₃ ; Na-NO ₃	Carbonate	SDW, SCW, BSW, SSW, NaCl
4	23.08	Na-NO ₃	Na-NO ₃	Sulfate	SSW, SAW, NaCl
5	44.23	Na-NO ₃	K-NO ₃ ; Na-NO ₃	Sulfate	SSW, SAW, NaCl
6	1.92	Na-Cl	K-NO ₃	Carbonate	SDW, SCW, BSW, SSW, NaCl

Source: ^a Table 6.10-6.^b Table 6.13-9.

NOTE: The probabilities represent the percentage of waste packages subject to dust that may deliquesce into the identified brine type.

6.13.6.3 Discussion of the Corrosion Test Solutions

The brine type name reflects a characteristic of the brine that distinguishes it from the other brines. When evaporation has gone beyond the classic chemical divides shown in Figure 6.2-1, it may no longer reflect dominant species in the brine. This characterization of surface brine types has in part guided the expected range of brine water chemistry in the repository. However, some differences are expected between brines formed at the earth's surface and brines formed in the repository. These differences are mainly due to differences in the chemistry of seepage waters and surface waters giving rise to brines, and differences between the salt chemistry of dust and the dissolved salt content of the surface waters. Two factors specific to the repository brines are the ubiquity of nitrate and more effective mechanisms for the removal of magnesium. It is expected that nitrate will be in these brines because of the multiple potential sources and the generally high solubility of nitrate minerals (BSC 2004 [DIRS 161237], Sections 6.7.2.8 and 4.1.7, and Table 4.1-9). It is expected that magnesium will not be significant because of limited sources (for the dust, as well as for at least some ground waters) and multiple removal mechanisms, most of which are enhanced by elevated temperature (BSC 2004 [DIRS 161237], Sections 6.7.2.10 and 6.7.2.11). Table 6.13-13 summarizes the general classification of the brine types that could be in contact with drip shields and waste packages and the probabilities of contact.

Table 6.13-13. General Classification of the Brine Types and the Probabilities of Contact

Brine Type	TSPA-LA Percent Probability		Comments
	Seepage at Drift Crown ^a	Dust Deliquescence ^b	
Calcium chloride	0.22	5.77 ^c	Fluoride, carbonate, sulfate contents are negligible
Sulfate	2.21	75.00	Near-neutral pH
Carbonate	97.56	19.23	High pH, no significant calcium or magnesium content

NOTE: ^aThe probability of crown seepage represents the 20,000-year time-integrated occurrence fraction of the representative water for each bin; at particular times in the simulation the bin probabilities may differ (Table 6.13-4). Additionally, the mapping from Table 6.13-11 for the 11 bins are as follows: Bins 1 to 3 are calcium chloride; Bins 4 and 5 are sulfate; and Bins 6 to 11 are carbonate.

^bThe probabilities represent the relative frequencies of occurrence for each dust type (bin). Additionally, the mapping from Table 6.13-12 is as follows: Bin 1 is calcium chloride; Bins 2, 4, and 5 are sulfate; and Bins 3 and 6 are carbonate.

^cAqueous solutions are dominated by $\text{Ca}(\text{NO}_3)_2$.

Calcium Chloride Brines—These brines may have acidic to near-neutral pH and no significant bicarbonate, carbonate, fluoride, or sulfate content. These brines may contain other cations such as Na^+ , K^+ , and Mg^{2+} and other anions such as NO_3^- . The endpoint of the evaporative concentration of this type of brine would contain Ca-Cl/NO_3 or a mixture of Ca/Mg-Cl/NO_3 . The quantity of Mg^{2+} and Ca^{2+} in this type of brine would be limited due to the precipitation of calcium carbonates and sulfates and magnesium silicates. This is consistent with information on saline lakes where Na^+ is the dominant cation with the percentage of Ca^{2+} varying from insignificant to about 20 percent (Drever 1997 [DIRS 147480]). In the repository, the concentration of Mg^{2+} in any type of brine is expected to be insignificant. Thus, a magnesium chloride brine is not expected. NO_3^- is expected to be present, and an end-point brine of this type is likely to be dominated by calcium chloride and calcium nitrate. A brine of the calcium chloride type is expected to have a very limited occurrence in the repository, as indicated in Table 6.13-13. For brine generated by dust deliquescence, the brine is actually expected to be more of a calcium-nitrate-sodium-chloride brine due to the compositional nature of the dust.

Relative humidity dependence of the calcium chloride brine is as follows. At low relative humidity, the aqueous solutions will be dominated by Ca^{2+} cations (very low sodium and potassium), and Cl^- and NO_3^- anions, since both calcium nitrate and calcium chloride are very soluble. At higher relative humidity, chloride and nitrate salts of sodium and potassium become soluble and could dominate the aqueous solution compositions. This would occur at or above the deliquescence relative humidity for salts composed of these ions.

Corrosion test solutions corresponding to this calcium chloride type of brine include: calcium chloride, calcium chloride plus calcium nitrate, the simulated saturated water (SSW) (Table 6.13-10), and sodium chloride aqueous solutions. The SSW and sodium chloride test solutions simulate the moderate relative humidity scenario where calcium is a minor component in the aqueous solution. Numerous electrochemical studies were performed in these test solutions. Thin film studies were also performed using these types of solutions on coupons of Alloy 22 using an environmental thermogravimetric analyzer.

Carbonate Brines—These brines are alkaline and do not contain significant calcium or magnesium. In the early stages of the evaporative concentration, calcium precipitates predominately as carbonate minerals (calcite or aragonite). Magnesium precipitates as a component in magnesium silicate (BSC 2004 [DIRS 161237], Section 6.7.2.11). In the repository, it is expected that magnesium will be removed efficiently, and potassium may be significant in some of these brines. As shown in Table 6.13-13, the carbonate brine is expected to be the most common type produced by evaporation of seepage water, and a minor type produced by dust deliquescence.

Relative humidity dependence of carbonate brine is as follows. At low relative humidity, the aqueous solutions will be dominated by Cl^- and NO_3^- anions with NO_3^- ions dominating at the lowest relative humidity. At moderate relative humidity (greater than 70 percent relative humidity) Cl^- could dominate the solution composition. The Cl^- - NO_3^- solutions are expected to have slightly elevated pH due to residual carbonate in solution. Significant amounts of carbonate and SO_4^{2-} are not expected until the relative humidity is greater than 85 percent.

Corrosion test solutions corresponding to the carbonate type of brine include: the simulated dilute water (SDW), simulated concentrated water (SCW), basic saturated water (BSW), and under certain circumstances SSW and simulated acidic water (SAW) aqueous test solutions (Table 6.13-10). The BSW test solution is a highly concentrated alkaline solution and could be expected under repository conditions where temperatures could be at its measured boiling point of nominally 112°C to 113°C or where the relative humidity is nominally 70 to 75 percent. The SCW test solution is a moderately concentrated alkaline solution; solutions in this concentration range could be expected to form for relative humidity in the range of 90 to 95 percent. The SDW test solution is a dilute alkaline solution; solutions in this concentration range could be expected to form for high relative humidity (greater than 99 percent). These may have characteristics of solutions at the drift wall, that is, typical of seepage waters.

Under conditions of extreme evaporative concentration (i.e., low relative humidity) the carbonate brine would evolve into a Cl^- - NO_3^- brine with low carbonate content. The SSW test solution has characteristics of this type of brine. Likewise the SAW test solution has characteristics of low carbonate brine and would have characteristics of solutions in equilibrium with relative humidity of nominally 90 percent. The calcium and magnesium content of the SAW test solution tends to make it more able to sustain lower pHs due to the hydrolysis properties of these cations.

Sulfate Brines—These have near-neutral pH and no significant carbonate or calcium content. Calcium precipitates as carbonates and possibly sulfates. In addition, brines typically have only a small amount of magnesium, though some surface brines have been observed to have high magnesium (Drever 1997 [DIRS 147480], Table 15-1, p. 333, brines 1-3). The dominant cation is typically Na^+ . In the repository brines, K^+ may be more significant than Na^+ , and Mg^{2+} is expected to be insignificant. As shown in Table 6.13-13, the sulfate-brine type is expected to be a minor type produced by evaporation of seepage water, but is expected to be contained in the dust.

Relative humidity dependence of the sulfate brine is as follows. At low relative humidity, the aqueous solutions will be dominated by Cl^- and NO_3^- anions, with NO_3^- ions dominating at the lowest relative humidity. At moderate relative humidity (greater than 70 percent relative

humidity) Cl^- ions could dominate the solution composition. However, unlike the carbonate brines these brines are expected to have near neutral to slightly acidic pH because of the lack of a carbonate component. Significant amounts of carbonate and SO_4^{2-} are not expected until the relative humidity is greater than 85 percent because of the increase in solubility of expected sulfate minerals (sodium and potassium sulfates). (Magnesium sulfate is expected to be present in only insignificant quantities in these repository brines.)

The corrosion test solutions corresponding to the sulfate type of brine include the SAW, SSW, and sodium chloride. This type of brine has near neutral to slightly acidic pH and as noted above magnesium is not expected to be present in seepage waters to any significant extent. The SAW test solutions have characteristics of solutions in equilibrium with nominally 90 percent relative humidity. The SSW has characteristics of water that have undergone evaporative concentration to the extent that sulfate precipitates out of solution (this is for the magnesium free situation). Sodium chloride test solutions simulate the scenario where Cl^- is the dominant anion under moderate relative humidity conditions.

6.14 FEATURES, EVENTS AND PROCESSES EVALUATION

Table 2 of the technical work plan (BSC 2004 [DIRS 171156]), lists the features, events, and processes (FEPs) related to the EBS physical and chemical environment as contained within the LA FEP list (DTN: MO0407SEPFELA.000 [DIRS 170760]).

The FEPs addressed in this document are listed in Table 6.14-1. In addition to the EBS FEPs listed here, several other FEPs that are explicitly incorporated in *Post-Processing Analysis for THC Seepage* (BSC 2004 [DIRS 169858], Table 6.1-1) are implicitly included in this analysis as part of model input (water and gas compositions) or boundary conditions. However, these additional FEPs are adequately addressed in *Post-Processing Analysis for THC Seepage* (BSC 2004 [DIRS 169858]) and are not repeated here.

Table 6.14-1. Included Features, Events, and Processes Addressed in This Report

FEP Number	LA FEP Title	Section Where Disposition is Described
2.1.08.06.0A	Capillary effects (wicking) in EBS	6.6, 6.9, 6.13
	Description: Capillary rise, or wicking, is a potential mechanism for water to move through the waste and EBS.	
2.1.08.07.0A	Unsaturated flow in the EBS	6.6, 6.9, 6.13
	Description: Unsaturated flow may occur along preferential pathways in the waste and EBS. Physical and chemical properties of the EBS and waste form, in both intact and degraded states, should be considered in evaluating pathways.	
2.1.09.01.0A	Chemical characteristics of water in drifts	6.4, 6.6, 6.7, 6.8, 6.9, 6.10, 6.12, 6.13
	Description: When flow in the drifts is reestablished following the peak thermal period, water may have chemical characteristics influenced by the near-field host rock and EBS. Specifically, the water chemistry (pH and dissolved species in the groundwater) may be affected by interactions with cementitious materials or steel used in the disposal region. These point source contaminated waters may coalesce to form a larger volume of contaminated water. This altered groundwater is referred to as the carrier plume because dissolution and transport will occur in this altered chemical environment as contaminants move through the EBS, and down into the unsaturated zone. ¹	

Table 6.14-1. Features, Events, and Processes Included in This Report (Continued)

FEP Number	LA FEP Title	Section Where Disposition is Described
2.1.09.02.0A	Chemical interaction with corrosion products	6.7, 6.8
	Description: Corrosion products produced during degradation of the waste form, metallic portions of the waste package, and metals in the drift (rock bolts, steel in invert, gantry rails) may affect the mobilization and transport of radionuclides. Corrosion products may facilitate sorption/desorption and coprecipitation/dissolution processes. Corrosion products may form a "rind" around the fuel that could (1) restrict the availability of water for dissolution of radionuclides or (2) inhibit advective or diffusive transport of water and radionuclides from the waste form to the EBS. Corrosion products also have the potential to retard the transport of radionuclides to the EBS. Finally, corrosion products may alter the local chemistry, possibly enhancing dissolution rates for specific waste forms, or altering radionuclide solubility.	
2.1.09.06.0B	Reduction-Oxidation potential in Drifts	6.7
	Description: The redox potential in the EBS influences the oxidation of the in-drift materials and the in-drift solubility of radionuclide species. Local variations in the in-drift redox potential can occur.	
2.1.09.07.0B	Reaction kinetics in Drifts	6.5, 6.6, 6.7, 6.8, 6.9, 6.10, 6.13
	Description: Chemical reactions, such as radionuclide dissolution/precipitation reactions and reactions controlling the reduction-oxidation state, may not be at equilibrium in the drifts.	
2.1.09.28.0A	Deliquescence on waste package outer surface	6.4, 6.7, 6.8, 6.10, 6.13
	Description: Salt-containing dust, which would have accumulated on the waste package surface during the preclosure ventilation period, can absorb moisture from the drift atmosphere, even at low RH, dissolving the salt and creating concentrated aqueous solutions. This deliquescence process may result in 1) moisture contacting the waste package surface earlier than predicted by general seepage and relative humidity considerations, 2) a localized surface chemistry that might be more corrosive than seepage waters or concentrated solutions created by evaporation of seepage waters.	
2.1.09.28.0B	Deliquescence on drip shield outer surface	6.4, 6.7, 6.8, 6.10, 6.13
	Description: Salt-containing dust, which would have accumulated on the drip shield surface during the preclosure ventilation period, can absorb moisture from the drift atmosphere, even at low RH, dissolving the salt and creating concentrated aqueous solutions. This deliquescence process may result in moisture contacting the drip shield surface earlier than predicted by general seepage and relative humidity considerations, and/or a localized surface chemistry that might be more corrosive than seepage waters or concentrated solutions created by evaporation of seepage waters.	
2.1.11.01.0A	Heat generation in EBS	6.7, 6.8, 6.9, 6.10, 6.12, 6.13
	Description: Temperature in the waste and EBS will vary through time. Heat from radioactive decay will be the primary cause of temperature change, but other factors to be considered in determining the temperature history include the in-situ geothermal gradient, thermal properties of the rock, EBS, and waste materials, hydrological effects, and the possibility of exothermic reactions. Considerations of the heat generated by radioactive decay should take different properties of different waste types, including DSNF, into account.	
2.1.11.08.0A	Thermal effects on chemistry and microbial activity in the EBS	6.4, 6.7, 6.9, 6.10,
	Description: Temperature changes may affect chemical and microbial processes in the waste and EBS.	

Table 6.14-1. Features, Events, and Processes Included in This Report (Continued)

FEP Number	LA FEP Title	Section Where Disposition is Described
2.2.08.04.0A	Redissolution of precipitates directs more corrosive fluids to waste packages	6.6, 6.9, 6.10, 6.13
	Description: Redissolution of precipitates which have plugged pores as a result of evaporation of groundwater in the dry-out zone, produces a pulse of fluid reaching the waste packages when gravity-driven flow resumes, which is more corrosive than the original fluid in the rock.	

NOTE: ¹There is no defining limit as to what volume of contaminated water constitutes a plume.

Table 6.14-2. Excluded Features, Events, and Processes Addressed in this Report

FEP Number	LA FEP Title	Section Where Disposition is Described
2.1.06.01.0A	Chemical effects of rock reinforcement and cementitious materials in EBS	6.4, 6.7, 6.8
	Description: Degradation of ground support material (cement, rock bolts, wire mesh) used for any purpose in the disposal region may affect long-term performance through both chemical and physical processes. Degradation may occur by physical, chemical, and microbial processes.	
2.1.06.05.0C	Chemical degradation of emplacement pallet	6.4, 6.7
	Description: Degradation of the materials used in the pallet supporting the waste package may occur by chemical or microbial processes, and may affect the long-term performance of the repository.	
2.1.06.05.0D	Chemical degradation of invert	6.4, 6.7
	Description: Degradation of the materials used in the invert may occur by chemical or microbial processes, and may affect the long-term performance of the repository.	

6.15 IMPLEMENTATION INSTRUCTIONS FOR TOTAL SYSTEM PERFORMANCE ASSESSMENT-LICENSE APPLICATION MODEL

This section describes how the chemistry and, more specifically, the lookup tables developed in Sections 6.6, 6.7, 6.9, and 6.10, and uncertainty instructions developed in Sections 6.12, are to be implemented in the TSPA-LA. This section provides roadmap figures for implementation of the lookup tables established in this report for the parameters of interest on the waste package surface and within the invert, during the development of the TSPA LA model. Although the processes used to ascertain these parameters for the two locations are similar, the resulting chemical environments are different.

A general rule that applies to the seepage scenarios discussed in the following subsection is that once a starting water is selected (i.e., w0, w4, w5, w6, or w7; Section 4.1.3), the associated $p\text{CO}_2$ gas lookup tables for that given water should also be selected for that given realization (Section 6.7.3.1). The TSPA-LA model should not select these two tables independently. This also means that the $p\text{CO}_2$ lookup table applied in the drift for waste package chemistry should be from the same starting water (e.g., w0, w4, etc.) as the selected crown seepage water entering the invert. In addition, the gas applied in the invert should be associated with the same starting water that is specified to select the gas in the drift. The only time that this rule does not apply is in the

dust deliquescence on the waste package surface scenario, because no seepage is present. In this case, any of the five $p\text{CO}_2$ lookup tables can be randomly selected for any given waste package.

6.15.1 Implementation of Engineered Barrier System Chemistry on Waste Package Surfaces

Two primary scenarios are envisioned for the use of the chemical parameters from the lookup tables on the waste package surface:

- When crown seepage is directly dripping onto the drip shields and waste packages
- When there is no seepage flowing onto the waste packages or drip shields and the deliquescent dust and salt minerals that have accumulated on the waste package surface absorb water due to the local relative humidity in the drift.

These two scenarios are independently discussed in the following subsection.

6.15.1.1 Seepage or "Dripping Scenario"

This scenario, in which crown seepage drips directly onto the waste package or drip shield surface, is modeled in the TSPA LA by using the roadmap given in Figure 6.15-1 and described further here.

For each TSPA LA realization, in order to represent the uncertainty of seepage water entering the drift, the starting water (w_0 , w_4 , w_5 , w_6 , and w_7 ; Section 4.1.3) must be randomly selected. All five of these waters have an equal probability of selection for any given TSPA LA realization. Therefore, the probability of any given water being selected is 20 percent.

Once the starting water is selected, the corresponding "bin history map" tables and associated $p\text{CO}_2$ lookup tables are selected. This map gives the bin history across time for that particular starting water (see Section 6.6 for the development of these maps). These "bin history map" tables are archived in DTN: MO0310SPAEBSCB.003 and are provided on Tables 6.6-8 through 6.6-12. The $p\text{CO}_2$ lookup tables are provided in Tables 6.7-1 through 6.7-5 and are archived in DTN: MO0308SPACO2GL.001. Each bin history map table and $p\text{CO}_2$ lookup table is unique to the particular starting water.

Next, for any given TSPA-LA model time step, the appropriate seepage water bin (Table 6.9-6 provides file names of lookup tables) and $p\text{CO}_2$ are determined (in the bin history map table, use the column labeled "Bin for Crown Seepage," and in each $p\text{CO}_2$ lookup table, use the column labeled "Drift"). Concurrently, temperature and relative humidity values for the same time step are obtained from other process models lookup tables.

The selected in-drift relative humidity value is used to determine whether the evaporation or dilution lookup tables are used. The dilution lookup tables are used if the selected relative humidity is greater than the relative humidity boundary condition values found in Table 6.9-7. In all other cases, the evaporative lookup tables are used. Table 6.9-6 lists the files that are part of DTN: MO0304SPACSALT.000, along with the 99 lookup tables for evaporative conditions and 99 lookup tables for dilute conditions. This DTN has been modified slightly for TSPA-LA

use (Section 8.2.1) resulting in a DTN for use in the TSPA-LA model archived in DTN: MO0310SPAPCEGS.000.

The lookup table file nomenclature is *??c#t%\$.xls.xls* where:

- “??” is the two-digit bin number (01, 02, 03, etc.)
- “#” is 2, 3, or 4 for fugacity of CO₂ equal to 10⁻², 10⁻³, or 10⁻⁴ bar, respectively
- “%” is 4, 7, or 1 for temperature equal to 40°C, 70°C, or 100°C, respectively
- “\$” is e or c for evaporation or dilution.

The chemistries from the lookup tables are shown in Section 6.9.4 and in Appendix B.

NOTE: The equal sign indicates that the bin map and pCO₂ lookup table have to be associated with the same seepage water type (w0, w4, w5, w6, or w7).

Figure 6.15-1. Roadmap for Total Systems Performance Assessment - License Application Implementation of Engineered Barrier System Chemistry on the Waste Package Surface Under the “Dripping Scenario”

To select the appropriate chemistry from a selected lookup table, the nearest drift relative humidity value row is used. When selecting chemical parameters that fall between lookup tables, the parameters should be estimated using linear interpolation on temperature and log linear for $p\text{CO}_2$ parameters. Chemistry values should be extrapolated for pH, I, Cl, and N if the $p\text{CO}_2$ exceeds the range of 10^{-4} to 10^{-2} bar, established in the lookup tables (up to 2×10^{-2} and down to 1×10^{-5} bar). This is based on the uncertainty results documented in Section 6.12.4.3. For temperatures above 100°C and below 40°C , interpolation may not be used and values should be extrapolated as the 100°C or 40°C lookup tables, respectively. Discussion of temperature values to justify this is found in Section 6.7.2.2. If the RH is greater than the highest value in the lookup tables, use the highest value. Additional discussion of the use of interpolation is included in Section 6.13.3. Implementation of uncertainty on any parameter should be done in accordance with the instructions found in Section 6.12.5.

Nonconvergence—The EQ3/6 calculation runs used to produce the seepage lookup tables did not always converge on the eutectic point associated with the deliquescence RH value for very low water to solute ratios (this occurs at relatively low RH values). An appropriately conservative method to deal with this limitation is to specify that aqueous conditions exist at all times when seepage is occurring, regardless of the in-drift RH. For TSPA-LA purposes, the selection of chemical parameters below the reported DRH in the lookup tables (row with lowest RH value on the lookup table) can be done, because the chemistries are conservative with respect to NO_3 (i.e., NO_3 should only increase with respect to Cl with decreasing RH due to the presence of the halite chemical divide). The basis for this modeling decision is illustrated in Figure 6.13-29, where at low RH the NO_3 concentration climbs in comparison to Cl ion, indicating that no matter where the DRH is predicted for the seepage, nitrate will continue to dominate the brine chemistry. The exception to this general rule is bin 1, where $\text{Ca}(\text{NO}_3)_2$ is precipitating and NO_3 is being removed from the aqueous system. This occurs around an RH of 20 percent. However, at lower RH values, the Cl: NO_3 ratio remains relatively constant because of the continued precipitation of halite and the lowest value taken from the lookup table will result in a conservative estimate of the Cl: NO_3 ratio.

Salt Separation—As indicated in Section 6.11.2: If the relative humidity on a waste package undergoing seepage should fall below 77% RH, halite salt separation is presumed to occur.

6.15.1.2 Deliquescence or “No Drip Scenario”

This scenario is to be modeled in the TSPA-LA using the roadmap in Figure 6.15-2.

Waste Package/Drip Shield Surface "No Drip Scenario"

Figure 6.15-2. Roadmap for Total Systems Performance Assessment - License Application Implementation of Engineered Barrier System Chemistry on the Waste Package Surface Under the "No Dripping Scenario"

The identical pCO_2 , temperature, and RH histories selected based on the starting water composition are utilized for these no drip scenarios per Section 6.15.1.1.

In the dust deliquescence abstraction, the range of dust leachate compositions is treated as uncertainty. In any given simulation, the dust bins are probabilistically sampled only once. This is conceptually similar to the seepage evaporation abstraction in which the range in starting water compositions is also treated as uncertainty. The choice for a single dust per realization is justified because although the dust samples collected underground at Yucca Mountain represent simultaneous heterogeneity, the effects of long-term forced ventilation during repository operations are expected to be spatially uniform. Treating the range of observed dust compositions as uncertainty in TSPA-LA avoids dilution of the differences in predicted dose consequences that are associated with the range. Sampling the dust bin upon each waste package, or group of packages, would lead to a more narrow range of long-term predicted dose consequences. Therefore the chosen method is considered the more cautious approach.

The dust leachate lookup tables are archived in DTNs: MO0310SPADLALT.001 and MO0310SPADLHTL.000 and the chemistries contained in them are shown in Section 6.10.7 and in Appendix C.

The lookup table file nomenclature is *d?c##%.xls.xls* where:

- “??” is the bin number (1, 2, 3, etc.)
- “#” is 2, 3, or 4 for fugacity of CO₂ equal to 10⁻², 10⁻³, or 10⁻⁴ bar, respectively
- “%” is 04, 07, 10, 12, or 14 for temperature equal to 40°C, 70°C, 100°C, 120°C, or 140°C, respectively.

Because atmospheric pressure conditions are imposed in the repository through all time, there are conditions under which no water can be present (the existence of an aqueous liquid would require pressurized conditions). In order to determine when deliquescence water can be present in the repository environment, the TSPA-LA model should check to see when the RH conditions are possible for water to be present. This is done by comparing the lookup table H₂O vapor pressure value against the value of atmospheric pressure at the repository level (0.89 bar). If the required pressure conditions of the chemistry are greater than this value, then no water can deliquesce until the RH rises (Figure 6.13-17). However, because of the uncertainty on deliquescence relative humidity (DRH), liquid water at or above 140°C is possible. The chemistry from the last data point on each of the 140°C lookup tables will be sufficient to predict the chemistry of the system in these sections of the lookup tables.

To select the appropriate chemistry from a lookup table, the nearest waste package relative humidity value row is used. When selecting chemical parameters that fall between lookup tables, the parameters should be estimated using linear interpolation on temperature and log linear interpolation on *p*CO₂ parameters. Chemistry values should be extrapolated for pH, I, Cl, and N if the *p*CO₂ exceeds the range of 10⁻⁴ to 10⁻² bar, established in the lookup tables (up to 2 × 10⁻² and down to 1 × 10⁻⁵ bar). This is based on the uncertainty results documented in Section 6.12. For temperatures above 140°C and below 40°C, no interpolation may be performed and values should be extrapolated as the 140°C or 40°C lookup table chemistry results respectively. If the RH is greater than the highest value in the lookup tables, use the highest value. Additional discussion of the use of interpolation discussion is included in Section 6.13.3. Implementation of uncertainty on any parameter should be done in accordance with the instructions found in Section 6.12.5.

The IDPS model predictions for DRH below 40 percent RH are outside the range of the IDPS model validation (Table 6.12-1). Therefore, for TSPA-LA purposes the dust on the waste packages should be considered wet at all times when the DRH (last value on the lookup table) occurs below 40 percent RH (without uncertainty applied). Even though the DRH is not a valid parameter at these low RHs, the solubility results from the lookup table are well within the appropriate IDPS model validation criteria and results (BSC 2004 [DIRS 169863]). Therefore, although the position of the final dryout point along the evaporative path is unknown, chemistries predicted at low RH are reasonable.

Dust Bins 2 through 6 can always be considered dry at or above 160°C, as per Assumption 5.2.2.

Dust Bin 1 should be considered wet at all times and temperatures. According to Table 6.12-1, the uncertainty in the DRH for $\text{Ca}(\text{NO}_3)_2$ also goes beyond the validation criteria established by the IDPS. Bin 1 is the only dust bin to precipitate $\text{Ca}(\text{NO}_3)_2$ (Table 6.13-7).

Selection of chemical parameters below the reported DRH in the lookup tables (row with lowest RH value on the lookup table) can be done, as these chemistries should be conservative with respect to NO_3 (i.e., NO_3 should only increase or remain constant with respect to Cl with decreasing RH due to the initial encounter with halite chemical divide). The basis for this modeling decision can be seen from Figure 6.13-38, where at low RH the NO_3 concentration climbs in comparison to Cl, indicating nitrate will continue to dominate the brine chemistry regardless of where DRH is predicted for the deliquescent dusts. One exception to this is the values in dust bin 1 (which contains the highest ratio of nitrate) below 70°C where soda niter is encountered prior to halite, precipitating NO_3 from the aqueous system. This occurs briefly around an RH of 60 percent, just before the halite divide is reached. In this case, the Cl: NO_3 ratio briefly increases and then remains relatively constant once the halite divide has been crossed.

6.15.2 Implementation of Engineered Barrier System Chemistry in the Invert

The following instructions are imposed to ensure that the appropriate parameters are selected for lookup tables (crown seepage or invert wicking) that may be used in the invert cell of the TSPA-LA model.

For each TSPA-LA realization, one of the five starting seepage waters (w0, w4, w5, w6, and w7) must be selected randomly. All starting waters are equally probable and, therefore, the probability of any given water being selected is 20 percent.

Once the starting water is selected, the "bin history map" (crown seepage and invert) and $p\text{CO}_2$ lookup tables (invert only) are used. There are two separate history maps, one for crown seepage and one for invert wicking water. These "bin history maps" are archived in DTN: MO0310SPAEBSCB.003 and can be found on Tables 6.6-8 through 6.6-12. The next set of lookup tables that are used is the $p\text{CO}_2$ lookup tables. The invert $p\text{CO}_2$ lookup tables are archived in DTN: MO0308SPACO2GL.001 and can be found on Tables 6.7-1 through 6.7-5. Whether the incoming water originates in the crown as seepage or from invert wicking, all evaluations of invert chemistry should apply the invert $p\text{CO}_2$ tables to select appropriate chemical values. The drift $p\text{CO}_2$ tables should not be used in the invert. Each bin history map table and $p\text{CO}_2$ lookup table is unique to a particular starting water.

Determination to use either the crown seepage or the invert imbibition history maps is made by the following determinations for two scenario classes:

- 1) For the nominal scenario class, utilize the invert history map if the sum of seepage or drift-wall condensation flux, or both, is less than or equal to $10^{-6} \text{ m}^3/\text{yr}$ (1 ml/yr) per waste package. Otherwise, use the crown seepage history map, as this water will easily displace imbibed water, which is slow to replenish.
- 2) For the seismic scenario class, in which separation of the drip shield has occurred, utilize the invert history map if the sum of seepage and drift-wall flux condensation is less than

or equal to 10^{-6} m³/yr per waste package. When there is seepage and/or drift-wall condensation without advective flow through the waste package, the crown seepage map is used; if there is advective flow through the waste package, then use chemistry from *In-Package Chemistry Abstraction* (BSC 2004 [DIRS 167621]).

Next, for any given TSPA-LA model time step, the appropriate water bin (Table 6.9-6 provides file names of lookup tables) and $p\text{CO}_2$ are to be selected. In addition, temperature and relative humidity input for the same time step, which is available from other process models lookup tables, must be selected.

The selected in-drift relative humidity value should be used to determine whether the evaporation or dilution lookup tables are to be used. The dilution lookup tables are to be used if the selected relative humidity is greater than the relative humidity boundary condition values found in Table 6.9-7. In all other cases, the chemistries on the evaporative lookup tables are to be used. Table 6.9-6 is part of DTN: MO0304SPACSAULT.000, along with the 99 lookup tables for evaporative conditions and 99 lookup tables for dilute conditions. This DTN has been modified slightly for TSPA-LA use (see Section 8.2.1 for discussion) resulting in a DTN for use in the TSPA-LA model archived in DTN: MO0310SPAPCEGS.000.

The lookup table file nomenclature is ??c#t%\$.xls.xls where:

- “??” is the two-digit bin number (01, 02, 03, etc.)
- “#” is 2, 3, or 4 for fugacity of CO_2 equal to 10^{-2} , 10^{-3} , or 10^{-4} bar, respectively
- “%” is 4, 7, or 1 for temperature equal to 40°C, 70°C, or 100°C, respectively
- “\$” is e or c for evaporation or dilution.

The chemistries from the lookup tables are shown in Section 6.9.4 and in Appendix B.

To select the appropriate chemistry from a lookup table, the nearest invert relative humidity value row is used. When selecting chemical parameters that fall between lookup tables, the parameters can be estimated using linear interpolation on temperature and log linear interpolation on $p\text{CO}_2$ parameters. Chemistry values can be extrapolated for pH, I, Cl, and N if the $p\text{CO}_2$ exceeds the range of 10^{-4} to 10^{-2} established in the lookup tables (up to 2×10^{-2} and down to 1×10^{-5} bar). This is based on the uncertainty results documented in Section 6.12. For temperatures above 100°C and below 40°C, no interpolation is allowed and values should be extrapolated directly as the 100°C or 40°C lookup tables. If the RH is greater than the highest value in the lookup tables, use the highest value. Additional interpolation discussion is included in Section 6.13.3. Implementation of uncertainty on any parameter should be done in accordance with the instructions found in Section 6.12.5.

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7. VALIDATION

This section summarizes the validation of the three abstraction models detailed in Section 6, and provides additional supporting analysis and information. Section 7.1 contains a point-by-point review of how validation criteria are met, for confidence-building activities performed during and after model development. The remaining Sections 7.2 through 7.7 describe the additional corroborative analysis.

Section 7.2.1 compares thermal-hydrological-chemical (THC) reactive transport seepage abstraction model results with the binning abstraction to ensure that the abstraction described in Section 6.6, as implemented in Section 6.9, represents the original THC model results with sufficient accuracy. Section 7.2.3 examines a suite of repository-horizon porewater chemistry to see how they "bin" in comparison with the five starting waters that are abstracted for use in TSPA-LA. Section 7.2.4 compares the dust deliquescence abstraction results with the original dust leachate analytical data from which it was developed to ensure the abstraction described in Section 6.10 represents the original data with sufficient accuracy.

Section 7.3 enhances the validation of the IDPS model by considering evaporation of mountain spring water to concentrated alkaline brine, which is similar to the intended use of that process model in this report.

Section 7.4 compares deliquescence point comparisons with predictions derived from model evaporations using the EQ3/6 Version 8.0 software with the *data0.ypr* Pitzer database (for high ionic strength calculations) to experimental data taken from the literature.

No future validation activities are required. The following validation criteria and activities described are sufficiently robust to give adequate confidence in the models.

7.1 MEETING VALIDATION CRITERIA

7.1.1 Confidence Building During Model Development

In order to establish the scientific basis and accuracy for intended use of the models, the following discussion reiterates the measures for confidence building during model development, and the criteria for implementation, as specified in the technical work plan (BSC 2004 [DIRS 171156], Sections 2.2.2.2 and 2.2.2.4) for Level II validation. A summary is provided for each measure and its criteria, describing the results achieved and documented in this report.

7.1.1.1 Seepage Evaporation 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:

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 seepage evaporation abstraction and the bases for their selection are covered in Section 4.1. For the seepage evaporation abstraction the

rationales for equilibrium modeling, for including or excluding precipitating minerals and trace elements, are documented in a technically defensible manner.

- The rationale for equilibrium modeling is documented in Sections 6.5.3 and 6.5.4, which provide background discussion, and 6.5.4.1, which specifies explicit, technically defensible criteria used for selecting mineral inclusion or exclusion, including kinetics.
- Mineral suppressions (i.e., including or excluding precipitating minerals) are documented in Section 6.12.4.4, which specifically evaluates the effects of minerals cryolite, glaserite, and magnesite on the results of the abstractions. The resulting shifts in abstraction model output are well within the model uncertainties associated with the IDPS model (changes less than one order of magnitude).
- The framework for evaluation of certain trace elements is documented in Section 6.5.4.2. Analysis of bromide (Section 6.12.4.2) shows that inclusion of bromide in the seepage evaporation abstraction, at concentrations related to the measurements on porewater s, would cause insignificant changes in output from the abstraction.

The rationale for including or excluding the chemical effects from ground support material degradation on water composition, is documented in Section 6.8, with additional sensitivity to background water chemistry, CO₂ fugacity, and Cr(VI) speciation provided in Section 6.12.4.1.

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)]

Discussion of the initial and boundary conditions for the seepage abstraction model are covered in Sections 4.1.3 and 6.6.1. For the seepage abstraction model, nonconvergence of EQ3/6 runs was encountered when calculating dryout (eutectic compositions) at very low water activity values (Section 6.15.1.1). The representation of nitrate and chloride concentrations for these conditions is based on known solubility of nitrate and chloride salts, and the abstraction provides a reasonable lower bound on the nitrate/chloride ratio.

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

For the seepage evaporation abstraction the predictive model uncertainty associated with use of the IDPS model is propagated to TSPA using uncertainty lookup tables, as described in Section 6.12.5. The statistical uncertainty inherent to binning of THC seepage model output waters into the 11 bins, is represented in binning uncertainty distributions that 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 seepage evaporation abstraction includes defensible assumptions (Section 5) and simplifications in model development (addressed in Sections 6.2, 6.5, and 6.12). The seepage evaporation abstraction maintains consistency with physical principles, such as conservation of mass and energy, through the use of EQ3/6 software (Section 6.5.1).

7.1.1.2 Dust Deliquescence 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 initial boundary conditions for the dust deliquescence abstraction is covered in Section 6.10. The rationales for equilibrium modeling, for including or excluding precipitating minerals, and for including or excluding trace elements, are the same as described above for the seepage evaporation abstraction. For dust deliquescence abstraction, transport is very limited and the time available for chemical changes is many years, which provides additional justification for equilibrium modeling. The presence of bromide as a trace constituent of dust is addressed in Section 6.12.4.2.

The selection of dust leachate analyses for the dust deliquescence abstraction is documented in a technically defensible manner in Section 6.10.2. Two of the 59 samples from Yucca Mountain are rejected as incomplete analyses, and three others are not representative of emplacement drift conditions.

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)]

Discussion of the initial and boundary conditions for the dust deliquescence abstraction is covered in Section 6.10. Nonconvergence of EQ3/6 calculations for the dust deliquescence abstraction occurred in the attempts to calculate the deliquescence relative humidity (Section 6.15.1.2) particularly for dust bin 1 (which is dominated by $\text{Ca}(\text{NO}_3)_2$). For such conditions the TSPA is instructed not to allow dryout, and bounding arguments are provided for use of the IDPS model results outside the validation range (i.e., at relative humidity less than 40%). These arguments are based on the known solubility behavior of nitrate and chloride salts, which dominate the solution chemistry in this range of environmental conditions.

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

For the dust deliquescence abstraction the predictive model uncertainty associated with use of the IDPS model, is propagated to TSPA using uncertainty lookup tables, as described in Section 6.12.5. The statistical uncertainty inherent to binning of dust leachate compositions into six bins is represented in binning uncertainty distributions that

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 169856], 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

lower fugacity limit to be 10^{-9} bars (BSC 2004 [DIRS 169863], Section 4.1.2). Two such comparisons are made: 1) comparison with the PO_2 values from the THC seepage model calculations, in which oxygen is not a reactant but is diluted by water vapor or steam (Section 6.7.2); and 2) comparison with a sensitivity analysis of oxygen consumption from degradation of introduced materials in the emplacement drifts (Section 6.7.1). The first comparison is discussed in Section 7.1.2.3. The results from the second comparison (Section 6.7.2) show that consumption of oxygen by degradation of steel decreases the fugacity, but that it is likely to remain greater than the lower limit stated above, supporting validation of the abstraction.

Documentation of the gas 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).

7.1.2 Confidence Building After Model Development

To support the scientific basis of the model, the following discussion reiterates the measures for confidence building after model development, and the criteria for implementation, as specified in the technical work plan (BSC 2004 [DIRS 171156], Sections 2.2.2.2 through 2.2.2.4) for the Level-II validation. A summary is provided for each measure and its criteria, describing the results achieved and documented in this report.

7.1.2.1 Seepage Evaporation 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. Meeting Validation Criteria for Post-Development Method 6: *Corroboration of abstraction model results to the results of the validated mathematical model(s) from which the abstraction model was derived.*

For the seepage evaporation abstraction, Method 6 is justified because the abstraction involves direct use of the input data from one of underlying mathematical models (i.e., the THC seepage model with selection of data in BSC 2004 [DIRS 169858]). The abstraction transforms this input using the IDPS model within its range of validation, with one qualification. Specifically, all the seepage evaporation abstraction calculations with the IDPS model are within the validation range, but predictions of deliquescence relative humidity (dryout) for relative humidity less than 40% are not permitted (BSC 2004 [DIRS 169863], Section 8.4). This situation is addressed by requiring that all such systems remain aqueous, and by applying the knowledge that nitrate behaves conservatively with respect to chloride for these conditions (Section 6.15.1.1). For relative humidity values less than 40 percent, the IDPS output is used in the abstraction (consistent with its validation), until the deliquescence relative humidity (dryout) is approached. At lower humidity values the IDPS model is not used for additional calculations, and the abstraction output consists of the last, near-dryout values from the IDPS supported by arguments based on the known behavior of nitrate and chloride. This

is a conservative approximation because it maintains the possibility of aqueous corrosion at humidity values less than the likely dryout condition.

Comparisons of the selected THC seepage model output with the corresponding, unmodified, median-bin waters are documented in Section 7.2.2 for the seepage evaporation abstraction. The unmodified waters are not evolved to the conditions of temperature, relative humidity, and $p\text{CO}_2$ that would most closely represent each output composition from the THC model. Rather, a simpler comparison is used in which the median-bin water starting point for such evolution at each time step is combined with the IDPS model uncertainty and the binning uncertainty, to show that the resulting ranges encompass the corresponding values in the five THC seepage model runs, for pH, nitrate, and chloride. Some exceptions are noted in Section 7.2.2, but these are relatively few and they are explained by the origins of the median-bin waters.

2. Meeting Validation Criteria for Postdevelopment Method 1: *Corroboration of model results with data acquired from the laboratory, field experiments, analog studies, or other relevant observations not previously used to develop or calibrate the model.*

The binning process in the seepage evaporation abstraction is evaluated using a sensitivity analysis in which the additional measured porewater compositions are processed in the same manner and compared to the binning of output from the THC seepage model (Section 7.2.3). One of the available 40 total porewaters was rejected from the analysis due to an unreasonable nitrate concentration of 0.0 mg/L (Section 7.2.3). The remaining 39 porewaters (including the five starting waters used in the THC seepage model) fall into bins 2, 3, 5 and 7. The additional porewaters are distributed among these bins in a manner similar to the five initial starting waters, as shown in Table 7.2-1. Further, most of the additional porewaters fall into bins 5 and 7, which are representative of the bins occupied by THC seepage model output waters at later times (compare Table 7.2-1 with Figure 6.13-1).

3. Meeting Validation Criteria for Postdevelopment Method 2: *Corroboration of results with alternative mathematical models.*

For the seepage evaporation abstraction, the binning process was compared to an alternative approach based on the precipitates formed during evaporation (Section 6.11.1). The overall clustering statistics (the overall mean of all coefficients of variation for all chemical constituents) is 26% for both the aqueous and mineral-based binning approaches. The mean coefficients of variation for individual analytes are all less than 50% except for calcium (Table 6.11-6). More important, equal numbers of analytes (six each) had lower variability for the aqueous binning and the mineral-based binning, meaning that neither approach is significantly better, corroborating the seepage evaporation abstraction approach.

The salt-separation effect can occur when environmental conditions cause precipitation of sodium chloride, but the residual aqueous phase is transported, leaving the salt on the surface of the drip shield or waste package. When humidity increases the salt can deliquesce, producing chloride-dominated aqueous chemistry. The possibility of this

alternative representation of the evolution of waters on the barrier surfaces is documented in Section 6.11.2, and the effect is implemented in TSPA as discussed in Section 6.15.1.1.

4. Meeting Validation Criteria for Postdevelopment Method 3: *Corroboration with information published in refereed journals or literature.*

Additional model-data comparisons supporting the application and validity of the IDPS model for describing the evaporative behavior of natural aqueous solutions in the in-drift environment are documented in Section 7.3. Close agreement of the IDPS model predictions with a widely known source (Garrels and Mackenzie 1967 [DIRS 123636], p. 239), which shows the evolution of a natural brine, is given in Figure 7.3-1. The published data, on which this comparison is based, were not used in development or validation of the IDPS model (BSC 2004 [DIRS 169863]).

The results described above show that a sufficient level of confidence in the seepage evaporation abstraction model has been achieved, to support Level-II validation for its intended use.

7.1.2.2 Dust Deliquescence 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. Meeting Validation Criteria for Postdevelopment Method 6: Corroboration of abstraction model results to the results of the validated mathematical model(s) from which the abstraction model was derived.

For the dust deliquescence abstraction, similar to the seepage evaporation abstraction, Method 6 is justified because the abstraction involves direct use of applicable measured data for dust leachate compositions. The measured compositions are compared to the model abstraction results for the TSPA-LA-relevant parameters in Section 7.2.4.

The abstraction transforms this input using the IDPS model within its range of validation, with two qualifications:

- i. All the dust deliquescence abstraction calculations using the IDPS model are within its validation range, but predictions of deliquescence relative humidity (dryout) for relative humidity less than 40% are not permitted (BSC 2004 [DIRS 169863], Section 8.4). This situation is addressed by requiring that all such systems remain aqueous, and by applying the knowledge that nitrate behaves conservatively with respect to chloride (Section 6.15.1.1). For relative humidity values less than 40%, the IDPS output is used in the abstraction, until the deliquescence relative humidity (dryout) is approached. At lower humidity values the IDPS model is not used to produce additional results, and the abstraction output consists of the last, near-dryout values from the IDPS, supported by arguments based on the known behavior of nitrate and chloride. This is a

conservative approximation because it maintains the possibility of aqueous corrosion at humidity values less than the likely dryout condition.

- ii. The upper temperature limit of the IDPS model validation is 140°C, and the dust deliquescence abstraction must provide key chemical parameters (deliquescence relative humidity, and nitrate/chloride ratio) to represent the corrosion environment at higher temperatures. This is done using two approximations, which are developed in Section 6.15.1.2: 1) all temperatures up to a limiting value, set at 160°C, with the exception of dust bin #1 which is aqueous at all temperatures; and 2) the composition of an aqueous phase above 140°C is represented only by the nitrate/chloride ratio, which is fixed at the 140°C value, supported by arguments based on the known behavior of nitrate and chloride.
2. Meeting Validation Criteria for Postdevelopment Method 3: Corroboration with information published in refereed journals or literature.

Comparisons of calculated vs. measured deliquescence relative humidity values for several relevant single-salt and mixed-salt systems are shown in Table 7.4-2, and the differences are on the order of 10% or less. These data represent the temperature-dependent deliquescent behavior of soluble salts and salt mixtures that are present in dust, as evident in the dust leachate compositions (i.e., compare the mineral assemblages in Table 7.4-2 with BSC 2004 [DIRS 161237], Section 6.7.2.10). The published data sets, on which these comparisons are based, were not used in development or validation of the IDPS model (BSC 2004 [DIRS 169863]).

The results described above show that a sufficient level of confidence in the dust deliquescence abstraction model has been achieved, to support Level-II validation for its intended use.

7.1.2.3 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. Meeting Validation Criteria for Postdevelopment Method 6: *Corroboration of abstraction model results to the results of the validated mathematical model(s) from which the abstraction model was derived.*

The gas abstraction consists of adopting $p\text{CO}_2$ time-histories directly from the underlying process model (the THC seepage model), and setting the oxygen fugacity to a constant (atmospheric) value representing oxidizing conditions, in accordance with the IDPS model (BSC 2004 [DIRS 169863], Section 8.4). No further validation is needed for the use of $p\text{CO}_2$ time-histories directly from the THC seepage model without modification.

For the oxygen fugacity part of the gas abstraction, the constant value of 0.21 bars is used in the abstraction to represent oxidizing conditions (in accordance with BSC 2004 [DIRS 169863], Section 8.4). 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 lower fugacity limit to be 10^{-9} bars (BSC 2004 [DIRS 169863], Section 4.1.2). Two sensitivity studies are used to evaluate this criterion: 1) the consumption of oxygen by corrosion of steel in the drift environment is addressed in Sections 6.7.1.1 and 6.7.1.2; and 2) the effect of dilution with water vapor (steam) is documented in Section 6.7.1.2 and summarized below.

The smallest partial pressure of oxygen (oxygen fugacity) that occurs at the drift wall, in any of the THC seepage model runs used for TSPA, has a value of approximately 6×10^{-6} bars, which is substantially greater than 10^{-9} bars (Section 6.7.2). This dilution effect is caused by displacement of air by water vapor at or near the peak of the thermal period. The result presented in Section 6.7.2 is conservative (overestimates dilution) because the THC seepage model is a two-dimensional cross-sectional model that does not consider the air and water vapor movement in the axial direction within the drift. This sensitivity analysis confirms the validity of the gas abstraction.

The results described above show that a sufficient level of confidence in the gas abstraction model has been achieved, to support Level-II validation for its intended use.

7.2 MODEL ABSTRACTION VALIDATION CASES

Three sets of abstraction comparisons are discussed in this section. The first set (Section 7.2.1) compares the binning abstraction to that of the THC seepage model output. The second comparison (Section 7.2.2) uses a set of lookup tables and performs an interpolation between the lookup tables in a similar manner as described in Sections 6.15.1.1 and 6.15.1.2. Section 7.2.3 examines all currently available and complete porewater chemistries and compares them to the five starting waters abstracted in this report. Lastly, Section 7.2.4 compares the binning dust leachate abstraction to the original set of dust leachate analytical data.

7.2.1 Comparison of THC Seepage Model with Seepage Evaporation Abstraction

In accordance with the defined criteria in Section 7.1, the seepage evaporation abstraction results are compared to the actual THC seepage model output results to insure that the original THC model output results are within the bounds of the abstraction uncertainty range.

These comparisons are documented in *THC Seepage Validation Spreadsheet LOG distributions.xls* (DTN: MO0312SPAPCESA.002), which contains the output values developed in Section 6.6. This spreadsheet was constructed using the THC Starting Chemistry Tables worksheet (copied from *Final Checked EBS THC Seepage Binning Abstraction REV 4.xls* archived in DTN: MO0310SPAEBSCB.003), the "All Data" worksheet and the 11 bin worksheets copied from *New Non Evaporated Binning Statistics.xls* archived in DTN: MO0310SPAEBSEUE.002.

For each comparison (Figures 7.2-1 through 7.2-11), two series of data and model uncertainty bars were plotted:

- First, the “THC Seepage,” the actual water chemistry found on the “all data” worksheet. These data are the THC model values of the waters identified (see Section 6.6.2) to potentially seep into the drift from the crown (“tf4”) or from the invert (“bf4”) for the various THC model starting waters (W0, W4, W5, W6, and W7). These values change as a function of time.
- Second, the “Bin Median Water Abstraction,” the median water chemistry parameter found on the “THC starting chemistry” tables. These are the median water compositions chosen for each of the 11 bins. The compositions do not change with time, rather, the bin assignment varies with time for each of the five starting waters. Importantly, as plotted in Figures 7.2-1 through 7.2-11, the median bin waters are not equilibrated to the extant environmental conditions in the drift (temperature, relative humidity, and fugacity of carbon dioxide) which do change with time. This simple approach to the comparison shows that reasonable correspondence with the THC model output is obtained without further detailed calculations, with a few exceptions discussed below. The differences between the median bin waters (with uncertainty) and the THC model output are not errors, but result mainly from not equilibrating the median waters with the environmental conditions associated with the THC model output.
- Third, the 2s log-uncertainty bars representing the binning uncertainty, i.e., the estimated uncertainty introduced in the abstraction (binning) process. The 2s values used to generate the log-uncertainty bars are twice the standard deviations calculated from the logs of the component concentrations in the abstracted THC seepage waters for each bin (Table 6.12-4). This 2s uncertainty estimate captures approximately 95 percent of uncertainty range. These binning uncertainty estimates are bin specific, but do not change as a function of time. The 2s values are applied to the “Bin Median Water Abstraction” in the figures to generate $\pm 2s$ log-uncertainty bars.

Figures 7.2-1 through 7.2-11 compare the median bin water compositions with the original THC model output. As an example, the abstraction bin information for Figure 7.2-6 is mapped in Figure 6.13-1 for water “W5” in the invert. The THC seepage water represents the temporal evolution of this water (matrix water at the base of the invert, for the wetting front at node four - W5bf4). To limit the comparisons to a reasonable number, the results for all five waters are shown only for crown seepage pH, Cl^- , and NO_3^- (Figures 7.2-1, 7.2-5, and 7.2-11). Plots for other solution parameters are provided for specific starting waters, selected as random examples (Figures 7.2-2 and 7.2-3, Ca^{2+} and Mg^{2+} for starting water W0; Figure 7.2-4, Na^+ for starting water W4; Figures 7.2-6 and 7.2-7, SiO_2 and HCO_3^- for starting water W5; Figures 7.2-8, and 7.2-9, SO_4^{2-} and K^+ for starting water W6; and Figure 7.2-10, F^- for starting water W7).

Uncertainty in the THC model abstraction is evaluated under normalized conditions in Section 6.12.

The abstraction, represented by the median bin water time histories and the binning uncertainty, provides a smoothed version of the THC model output. With the exception of a few data, all the

THC model output values plotted lie within the 2s log-uncertainty bars. The correspondence would be much closer, particularly for those THC model results that fall outside the uncertainty bars, if the median bin waters for each point in time were equilibrated to the extant conditions of temperature, relative humidity, and carbon dioxide fugacity associated with the THC model values.

One exception is the apparent underprediction of Cl^- and NO_3^- concentrations at approximately 53 years (Figures 7.2-5 and 7.2-11), which is due to evaporative concentration (i.e., lower relative humidity) that is explicitly included in the THC model but not accounted for in the treatment of median bin waters for these figures. Importantly, for the implementation of the seepage evaporation abstraction in TSPA (and also the dust deliquescence abstraction), the median bin waters are equilibrated to the extant conditions of temperature, relative humidity, and carbon dioxide fugacity.

Another exception is noted in the pH (Figure 7.2-1, a through d) at about 2,000 years when the time series of median bin waters does not represent the transient pH decrease. The cause is that, except for water W7, the median bin water for bin 4 is assigned to this time step (see Tables 6.6-8 through 6.6-12 at starting year of 1,901). The bin-4 median water actually originates from the THC model output at 600 years, when the CO_2 level is lower (4.8×10^{-4} bars). Comparatively, at 2,000 years the CO_2 level is increased significantly to approximately 6.5×10^{-3} bars (see Tables 6.7-1 through 6.7-5 at starting year of 1,901.5). The increase in CO_2 fugacity (approximately one order of magnitude) if used in equilibration of the bin-4 median water, would decrease the pH of the bin-4 median water to a similar extent.

(To obtain this result, a hand-interpolation can be done using the lookup tables for bin 4 at 100°C: files *04c2tlc.xls* and *04c3tlc.xls* found in *seepage_lookup_cond.zip* in output DTN: MO0310SPAPCEGS.000. For the bin-4 median water, the pH is 7.155 and 7.674 for CO_2 at 10^{-2} and 10^{-3} bars, respectively. Interpolating this by the log-scale value for CO_2 at 2,000 years, $6.5 \times 10^{-3} = 10^{-2.2}$, produces a pH value of 7.26. This is significantly lower than the unadjusted median pH of 7.90 for bin 4, and it encompasses the pH values from the THC model output at 2,000 years in Figure 7.2-1.)

As stated previously, the comparisons in Figures 7.2-1 through 7.2-11 show that reasonable correspondence with the THC model output is obtained, with a few exceptions, without further detailed calculations. Not only would the comparisons improve with equilibration of the median bin waters, but the in-drift precipitates/salts (IDPS) model uncertainty (Section 6.12.3.1 and Table 6.12-1) should be added to the median bin water compositions (to represent how these measures are formulated in TSPA). The magnitude of the IDPS model uncertainty is generally 1 pH unit for temperatures less than boiling, and ranges from zero to 0.2 log-units for Cl^- concentration and the $\text{Cl}^-/\text{NO}_3^-$ molar ratio. The IDPS model uncertainty implemented in TSPA further improves the comparisons as they are represented in Figures 7.2-1 through 7.2-11, and especially for pH (Figure 7.2-1).

Based on the comparisons discussed above, reasonable correspondence is shown between the seepage evaporation abstraction and the THC model output, without further detailed calculations. Further discussion of uncertainty in the seepage evaporation abstraction model, and how it is implemented in TSPA, is presented in Section 6.12.

Figure 7.2-1. Comparison of Thermal-Hydrological-Chemical Seepage pH with Crown Seepage Water Abstraction Results

Source: Output DTN: MO0312SPAPCESA.002.

Figure 7.2-2. Comparison of Thermal-Hydrological-Chemical Seepage Ca²⁺ with Abstraction Results for w0bf4

Source: Output DTN: MO0312SPAPCESA.002.

Figure 7.2-3. Comparison of Thermal-Hydrological-Chemical Seepage Mg²⁺ with Abstraction Results for w0tf4

Source: Output DTN: MO0312SPAPCESA.002.

Figure 7.2-4. Comparison of Thermal-Hydrological-Chemical Seepage Na⁺ with Abstraction Results for w4bf4

NOTE: Cl^- units given as log Molarity.

Figure 7.2-5. Comparison of Thermal-Hydrological-Chemical Seepage Cl^- with Crown Seepage Water Abstraction Results

Figure 7.2-6. Comparison of Thermal-Hydrological-Chemical Seepage $\text{SiO}_2(\text{aq})$ with Abstraction Results for w5bf4

Figure 7.2-7. Comparison of Thermal-Hydrological-Chemical Seepage HCO_3^- with Abstraction Results for w5tf4

Source: Output DTN: MO0312SPAPCESA.002.

Figure 7.2-8. Comparison of Thermal-Hydrological-Chemical Seepage SO_4^{2-} with Abstraction Results for w6bf4

Figure 7.2-9. Comparison of Thermal-Hydrological-Chemical Seepage K^+ with Abstraction Results for w6bf4

Source: Output DTN: MO0312SPAPCESA.002.

Figure 7.2-10. Comparison of Thermal-Hydrological-Chemical Seepage F^- with Abstraction Results for w7bf4

NOTE: NO_3^- units given as log Molarity.

Figure 7.2-11. Comparison of Thermal-Hydrological-Chemical Seepage NO_3^- with Crown Seepage Water Abstraction Results

7.2.2 Comparison of Lookup Table Interpolations with P&CE Model Results

In accordance with the validation criteria (Section 7.1), the lookup table interpolation results are compared with an actual THC model output to ensure that the interpolation results are within the bounds of the uncertainty range on the actual model output.

The inputs selected for this validation calculation were from Bin 11 seepage lookup table EQ6 calculations found in DTN: MO0304MWDEBSSA.000. These include the following input and output files:

- *11c3t4e.6i*
- *11c3t7e.6o*
- *11c3t4e.6o*
- *11c4t7e.6o*
- *11c4t4e.6o*

The input file *11c3t4e.6i* was modified to replace the temperature and CO₂ partial pressure and renamed *bin11val.6i*. The selected temperature and $p\text{CO}_2$ for the actual model calculation run was 56°C and $10^{-3.2}$ bars of CO₂.

Software application EQ3/6 version 8.0 was used to run *bin11val.6i* along with *Data0.ypf* (DTN: SN0302T0510102.002 [DIRS 162572]) to create *bin11val.6o*. GetEQData was then used to extract the results from *bin11val.6o* along with the results of the four lookup table output files listed above into *bin11val.xls*.

In the validation, values for pH, ionic strength, Cl and NO₃ were first interpolated with respect to CO₂ partial pressure at 40°C and 70°C, and then the two nearest temperatures in the set of lookup tables. Interpolation for $10^{-3.2}$ bars of CO₂ partial pressure is accomplished by linearly interpolating the logarithms of CO₂ partial pressure. In this case, the two nearest logarithms of CO₂ partial pressure in the lookup tables are -3 and -4. The interpolated values were then plotted at 40°C and 70°C and connected by a straight line to determine the interpolated value at 56°C and $10^{-3.2}$ bars of CO₂. These interpolations generally show no variation in the parameters with temperature, excepting the NO₃, and their interpolations are, therefore, nearly identical to exact model results.

For NO₃, Figure 7.2-12 shows that even with dependence upon both carbon dioxide and temperature, the exact value (green square) is very well represented by the interpolated value at 56°C (red line), with the error bar nearly encompassing the entire range bound by the various carbon dioxide pressures and temperatures. The uncertainty data for the error bars are taken from Table 6.12-1; the files can be found in output DTN: SN0406T0510102.015.

Source: Output DTN: SN0406T0510102.015.

Figure 7.2-12. Comparison of Model Results (NO_3^- at 64% RH) with Lookup Table Interpolation Values

The actual model results when compared to the interpolation results indicate that the interpolated values fall well within the model uncertainty and are in fact almost identical to the actual model results. This indicates that the interpolation method performed in this validation provides adequate representation of the water chemistries using discrete lookup table results.

7.2.3 Binning of Repository-Horizon Porewaters

A binning analysis, similar to those in Section 6.6, of 40 measured repository-horizon porewaters was carried out to evaluate the range in brines that occur during their evaporation to 65 percent RH at 25°C. The resulting outputs for the EQ3/6 evaporation results (to 65 percent RH) were extracted from the input .6i files (archived in the output DTN: MO0406MWDARHPW.000) using GETEQDATA V1.0.1 (STN: 10809-1.0.1-00 [DIRS 161900]). These output are given in *Binning of Repository Horizon Pore Waters.xls* (archived in output DTN: MO0406MWDARHPW.000), which were then subjected to the binning analysis located in Section 6.6.

It is notable that most of the source DTNs for these porewater chemistries state that there are problems with the measured bicarbonate concentrations, indicated by the poor charge balancing. In at least one case, the statement is made that the measured values have been replaced in the data set with values calculated by charge balance—however, both values are actually presented in the table. In all cases, the measured values, which are stated to be suspect (or bad) in DTNs: GS020408312272.003 [DIRS 160899] and GS020808312272.004 [DIRS 166569], are used in the EQ3 input files. This, however, is irrelevant because charge balancing was done

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 169856], 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 169856]) are a good representation of the range in near-field chemistries that are reasonably present.

Table 7.2-1. Binning Distribution of Repository-Horizon Porewaters

Bin Number	Number of Porewaters in Each Bin	% Distribution	Number of THC Model Starting Waters ^a
2	2 ^b	5.3	1
3	3	7.9	0
5	14	36.8	2
7	19	50.0	2

Source: Output DTN: MO0406MWDARHPW.000; *Binning of Repository Horizon Porewaters.xls*; except "% Distribution" as hand calculation.

NOTES: ^a See Section 6.6 for the five THC starting waters.

^b THC model starting water "w0" would fall into bin 2, but since it was developed using the average chemistries of two repository-horizon waters that both included in this analysis, it is not included in columns 2 (Number of Porewaters in Each Bin) and 3 (% Distribution) to avoid double-counting of this water.

One THC water ("w0") is distributed in bin 2, but not included in the binning distribution in Table 7.2-1 because it is the average composition of the two measured waters that are included in the binning analysis (Table 7.2-1, Note *b*). Those two waters are distributed one into each of bin 2 and bin 3.

7.2.4 Comparison of Dust Leachate Analysis to the Dust Deliquescence Abstraction

In accordance with the defined criteria in Section 7.1, the dust deliquescence abstraction results are compared to the actual dust leachate analysis results to insure that the original output results are within the bounds of the abstraction uncertainty range.

For each comparison, experimental data, abstraction median, and bin uncertainty bars are plotted (Figures 7.2-13 through 7.2-15):

- First, the original dust leachate water chemistries are represented by the small black dots. These are modified only to bring the solution into charge balancing on pH and equilibrium to remove any supersaturation (primarily calcite); no evaporative concentration is included. The data for these points are obtained from output DTN: SN0310T0510102.010 and all the .60 output files from the "Evap" directory. It is the first output iteration block in these files that gives the information presented.
- Second, the median leachate composition for each bin is shown as a large red diamond. These are the dust leachate compositions chosen to represent each of the bins.
- Third, the 2s log-error bars representing the error introduced in the abstraction (binning) process. The 2s values used to generate the log-error bars are twice the standard deviations calculated from the log of the set of dust deliquescence abstraction in each bin (Table 6.12-8), this should then encompass approximately 95 percent of uncertainty range. Thus, these values are bin-specific, and do not change as a function of time, temperature, relative humidity, or fugacity of carbon dioxide. These 2s values are applied to the abstraction's bin median results in the figures. These error bars should not

be interpreted as complete uncertainty in the dust abstraction as they do not include modeling uncertainty.

Figures 7.2-13 through 7.2-15 compare the dust deliquescence abstraction, with uncertainty, to the original dust leachate analysis data. The results for five bins are shown, for pH, $\log(\text{Cl})$ and $\log(\text{Cl}/\text{NO}_3)$. Dust deliquescence bin 6 is not included in these figures as it consists of only a single dust sample, and therefore is exactly represented in the abstraction by the analyzed composition, with no uncertainty.

For these comparisons the error bars for the abstraction (in red) consist of the larger of binning uncertainties (2s) computed at 85 percent and 98 percent *RH* (Section 6.12.3). Thus EQ3/6 calculations of equilibrated composition at reference conditions, are compared to the original measured data at sampling conditions, which are not the same (Figure 7.2-14). The comparison is non-normalized and used in this report for expository purposes only. Uncertainty in the dust deliquescence model abstraction is evaluated under normalized conditions in Section 6.12.

The graph of the $\log(\text{Cl}/\text{NO}_3)$ is not generally affected by variation in concentration factor as both species are conservative for all but the most concentrated solutions. Thus, Figure 7.2-15 shows the best representation of the dust abstraction results to the original data set, and the binning uncertainty as defined encompasses all but three (of 52) data points.

Based on comparisons of this type, the abstraction is considered a valid representation of the dust leachate chemical results.

Source: DTNs: MO0310SPADLBU4.001 (*EBS Dust Leachate Binning Abstraction Rev 01.xls*) and SN0310T0510102.010 (all *.3o files), and Table 6.12-8.

Figure 7.2-13. Comparison of pH for the Median Leachate Composition for Each Dust, Including Uncertainty, to the Original Data

Source: DTNs: MO0310SPADLBU4.001 (*EBS Dust Leachate Binning Abstraction Rev 01.xls*) and SN0310T0510102.010 (all *.3o files), and Table 6.12-8.

Figure 7.2-14. Comparison of the log of Chloride Concentration for the Median Leachate Composition for Each Dust Bin, Including Uncertainty, to the Original Data from Leachate Analysis

Source: DTNs: MO0310SPADLBU4.001 (*EBS Dust Leachate Binning Abstraction Rev 01.xls*) and SN0310T0510102.010 (all *.3o files), and Table 6.12-8.

Figure 7.2-14. Comparison of the log of Chloride to Nitrate Ratio for the Median Leachate Composition for Each Dust Bin, Including Uncertainty, to the Original Data

7.3 EVAPORATION OF SIERRA NEVADA SPRING WATERS TO FORM CONCENTRATED BRINES

The process underlying the seepage abstraction model can be evaluated by comparison with alternative classical models, which employ evaporative concentration of dissolved species in solution (including precipitation). This comparison of an external natural water model to our model adds confidence to our seepage abstraction by demonstrating that the underlying evaporation modeling is sufficiently accurate. This example is the classical study of the isothermal evaporation, at 25°C and $p\text{CO}_2 = 10^{-3.5}$ bars, of Sierra Nevada spring waters by Garrels and Mackenzie (1967 [DIRS 123636], pp. 222 to 242), which has been cited by Drever (1988 [DIRS 118564], pp. 232 to 234), as “a simulation of what might happen if streams from the Sierra Nevada flowed out into one of the arid basins of Nevada” to form saline lake water.

Drever (1988 [DIRS 118564], p. 233) suggests that the resulting brine “chemistry of these lakes could be explained by simple evaporation of dilute spring waters whose chemistry was, in turn, controlled by reactions between rainwater and igneous rock.” In an analogous way, several Yucca Mountain waters can concentrate into alkaline carbonate brines by evaporation of initial crown seepage, invert wicking, or condensate that has reacted with volcanic tuff. It is useful to explore the similarities and differences between this classical study’s graphical display of pH and major ions as a function of up to 1,000-fold evaporation concentration against the same concentration range developed using the methodology of the present work (Figure 7.3-1).

Before detailing the results of the Sierra Nevada Spring evaporation calculations, the difference in databases, mineral suppression during speciation calculations, and the number of chemical species is evaluated. Garrels and Mackenzie (1967 [DIRS 123636], p. 234) originally considered 11 major aqueous species and seven minerals that could precipitate during evaporative concentration: calcite, gypsum, brucite, magnesite, hydromagnesite, sepiolite, and amorphous silica.

In this validation, up to 22 aqueous species whose concentrations were greater than 10^{-20} molal are output (this concentration limit is set in the EQ3/6 input files, *sierra.3i* and *sierra.6i*, archived in DTN: SN0404T0510102.014). Saturation values for nearly 40 minerals, minus mineral suppressions, are evaluated.

Further, the molecular formula of sepiolite and hydromagnesite has been revised. Sepiolite’s common molecular formula has been changed from $\text{MgSi}_3\text{O}_6(\text{OH})_2$ (Garrels and Mackenzie 1967 [DIRS 123636], p. 234) to $\text{Mg}_4\text{Si}_6\text{O}_{15}(\text{OH})_2 \cdot 6\text{H}_2\text{O}$ and hydromagnesite’s common molecular formula has been changed from $\text{Mg}_4(\text{CO}_3)_3(\text{OH})_2$ (Garrels and Mackenzie 1967 [DIRS 123636], p. 234) to $\text{Mg}_5(\text{CO}_3)_4(\text{OH})_2 \cdot 4\text{H}_2\text{O}$. The Debye-Huckel activity coefficients used by Garrels and Mackenzie are accurate up to an ionic strength of 0.05 molal (Garrels and Christ 1990 [DIRS 144877], p. 64). However, at the concentration factor of 1000 the ionic strength is nearly 0.2 molal (*sierra.6o* at 0.996 activity of water, archived in DTN: SN0404T0510102.014). Garrels and Mackenzie (1967 [DIRS 123636], p. 240) were aware of the problem in using activity coefficients derived for use in lower ionic strength solutions, and emphasized that using their results carried increasing uncertainty with ionic strength: “Using the Debye-Huckel activity coefficients obviously leads to an increasing uncertainty in γ_i (activity coefficient) values with increasing ionic strength, and the values

calculated for 1,000× concentration should be regarded as rough approximations.” The Pitzer activity coefficients calculated with the current modeling are accurate well over 1.0 molal.

Sources: Model: Output DTN: SN0404T0610102.014; Garrels and Mackenzie 1967 [DIRS 123636], p. 239.

NOTES: pptes = precipitates.

Mineral pptes labels and associated arrows do not necessarily indicate the location on the figure where precipitation begins, but rather indicate that the specific aqueous species that the arrow points to is controlled by the precipitation of the corresponding mineral that is given next to the arrow.

Figure 7.3-1. Comparison of Results of Evaporation of Typical Sierra Nevada Spring Water at 25°C in Equilibrium with Atmospheric $p\text{CO}_2$ at $10^{-3.5}$ bar

Figure 7.3-1 shows remarkable similarity despite the differences in how the literature and model results were derived. The evaporative concentration starts with a near neutral pH, Na-Ca-HCO₃ water and concentrates it to highly alkaline Na-HCO₃-CO₃ water. Calcium and magnesium are removed by early mineral precipitation of calcite and sepiolite, respectively. Na⁺, K⁺, Cl⁻, and SO₄²⁻ are conservatively concentrated without forming solids. Bicarbonate and carbonate ions deviate from log-linear concentration due to calcite precipitation and their equilibrium relation. Because the Sierra Spring waters are originally low in SO₄²⁻, gypsum doesn't precipitate. Aqueous silica is seen to saturate at approximately the same concentration, around 0.002 molal. Many waters in the repository are expected to concentrate by evaporation in a similar manner (Section 6.9).

The only difference lies in the initial concentration of chloride. This is only because of a difference in charge balancing between the literature and the validation modeling calculation. The validation modeling calculation performed charge balancing upon chloride, whereas the literature source utilized bicarbonate. As chloride is conservatively concentrated in both models (chloride never saturates with respect to any mineral or salt) this has a negligible impact upon the other species' comparisons.

The plotted data comparison of this report's model to Garrels and Mackenzie (1967 [DIRS 123636], pp. 222 to 242) validates the initial portion of an evaporative concentration of groundwater by corroboration with this natural analogue.

7.4 DELIQUESCENT POINT COMPARISON

Literature experimental corroboration of the process used to implement the dust deliquescence abstraction is presented here. This comparison of external deliquescence data to our model adds confidence to our deliquescence abstraction by demonstrating that the underlying modeling is sufficiently accurate to represent the process. The modeled equilibrium salt deliquescence points are comparing predictions made by the use of the EQ3/6 software with the *data0.ypf* Pitzer database, and experimental data for simple and mixed electrolytes reported by Greenspan (1977 [DIRS 104945]) and Pabalan et al. (2002 [DIRS 163067]). Greenspan (1977 [DIRS 104945]) presents a compilation of equilibrium relative humidity values for binary salts as a function of temperature. Pabalan et al. (2002 [DIRS 163067]) reports salt deliquescence point experiments for selected binary and mixed salts as a function of temperature. This validation effort follows the criteria defined in Section 7.1.

Each validation run predicts a water activity (equivalent to relative humidity) at the deliquescence point for a set of highly soluble salts within a temperature range of 23°C to 86°C. In the EQ3/6 calculation runs, the salt deliquescence point corresponds to the equilibrium of the electrolyte solution with respect to the salt solid. At this equilibrium point, EQ3/6 calculates the activity of water (or relative humidity) using the Pitzer activity model. The selected simple and mixed salt compositions for which deliquescence data are considered in the validation are NaNO₃, MgCl₂, NaCl + NaNO₃, and NaCl + NaNO₃ + KNO₃.

Input and output files used in the EQ3/6 calculations are listed in Table 7.4-1. The computed equilibrium relative humidity values for a given salt composition using the EQ3/6 and the *data0.ypf* Pitzer databases are given as a function of temperature in Table 7.4-2.

Table 7.4-1. Input/Output Files EQ3/6 (Version 8.0) Used to Calculate the Equilibrium Deliquescence Points of Binary and Mixed Salts

Temperature (°C)	Salt Composition	EQ3/6 (Version 8.0) Input Files	EQ3/6 (Version 8.0) Output Files
23	CaCl ₂	CaCl2_23.3i	CaCl2_23.3o
38.1	CaCl ₂	CaCl2_38.3i	CaCl2_38.3o
48	CaCl ₂	CaCl2_48.3i	CaCl2_48.3o
69	CaCl ₂	CaCl2_69.3i	CaCl2_69.3o
85.8	CaCl ₂	CaCl2_86.3i	CaCl2_86.3o
23	MgCl ₂	MgCl2_23b.3i	MgCl2_23b.3o
38.1	MgCl ₂	MgCl2_38b.3i	MgCl2_38b.3o
48	MgCl ₂	MgCl2_48b.3i	MgCl2_48b.3o
69	MgCl ₂	MgCl2_69b.3i	MgCl2_69b.3o
85.8	MgCl ₂	MgCl2_86b.3i	MgCl2_86b.3o
23	NaNO ₃	NaNO_23b.3i	NaNO_23b.3o
38.1	NaNO ₃	NaNO_38b.3i	NaNO_38b.3o
48	NaNO ₃	NaNO_48b.3i	NaNO_48b.3o
69	NaNO ₃	NaNO_69b.3i	NaNO_69b.3o
85.8	NaNO ₃	NaNO_86b.3i	NaNO_86b.3o
23	NaCl + NaNO ₃	naclno3_23.3i	naclno3_23.3o
38.1	NaCl + NaNO ₃	naclno3_38.3i	naclno3_38.3o
48	NaCl + NaNO ₃	naclno3_48.3i	naclno3_48.3o
69	NaCl + NaNO ₃	naclno3_69.3i	naclno3_69.3o
85.8	NaCl + NaNO ₃	naclno3_86.3i	naclno3_86.3o
23	NaCl + NaNO ₃ + KNO ₃	nakclno3_23.3i	nakclno3_23.3o
38.1	NaCl + NaNO ₃ + KNO ₃	nakclno3_38.3i	nakclno3_38.3o
48	NaCl + NaNO ₃ + KNO ₃	nakclno3_48.3i	nakclno3_48.3o
69	NaCl + NaNO ₃ + KNO ₃	nakclno3_69.3i	nakclno3_69.3o
85.8	NaCl + NaNO ₃ + KNO ₃	nakclno3_86.3i	nakclno3_86.3o
23	NaCl + NaNO ₃ + KNO ₃	nakclno3_23.3i	nakclno3_23.3o
38.1	NaCl + NaNO ₃ + KNO ₃	nakclno3_38.3i	nakclno3_38.3o
48	NaCl + NaNO ₃ + KNO ₃	nakclno3_48.3i	nakclno3_48.3o
69	NaCl + NaNO ₃ + KNO ₃	nakclno3_69.3i	nakclno3_69.3o
85.8	NaCl + NaNO ₃ + KNO ₃	nakclno3_86.3i	nakclno3_86.3o

Source: Output DTN: SN0303T0510102.004.

Table 7.4-2. Comparisons of Relative Humidity Values for Equilibrium Deliquescence Points of Selected Salts Between EQ3/6 (Version 8.0—*data0.ypr* Pitzer Database) and Experimental Data

Salt Composition	Code or Source	Temperature (°C)					EQ3/6 vs. Others: Percent Difference (Temperature) ^a
		23.0	38.1	48.0	69.0	85.8	
NaNO ₃	EQ3NR/EQ6 (Version 8.0)	74.3	70.8	68.6	64.3	61.1	—
	Greenspan (1977 [DIRS 104945])	74.7	71.4	69.4	66.2	65.0	-0.5(23), -0.8(38.1), -1.1(48), -2.9(69), -6(86)
	Pabalan et al. (2002 [DIRS 163067])	74.9	—	69.7	62.7	—	-0.8(23), -1.6(48), -2.5(69)
MgCl ₂ ^b	EQ3NR/EQ6 (Version 8.0)	37.0	35.8	34.8	31.9	28.4	—
	Greenspan (1977 [DIRS 104945])	32.9	31.8	30.8	27.9	25.0	12.5(23), 12.6(38.1), 13(48), 14.3(69), 13.6(86)
	Pabalan et al. (2002 [DIRS 163067])	33.9	31.7	31.0	29.1	—	9.1(23), 12.9(38.1), 12.3(48), 9.6(69)
NaCl + NaNO ₃	EQ3NR (Version 8.0)	68.7	66.9	65.6	62.7	60.1	—
	Pabalan et al. (2002 [DIRS 163067])	74.7	66.4	67.2	59.6	56.0	-8.0(23), -0.7(38.1), -2.4(48), 5.2(69), 7.3(86)
NaCl + NaNO ₃ + KNO ₃ ^c	EQ3NR/EQ6 (Version 8.0)	66.2	61.4	57.5	48.0	39.0	—
	Pabalan et al. (2002 [DIRS 163067])	67.8	60.7	61.3	51.8	43.4	-2.4(23), 1.1(38.1), -6.2(48), -7.3(69), -10.1(86)

Source: Output DTN: SN0303T0510102.004

^a Numbers represent percent difference, those in parenthesis represent temperature.^b MgCl₂ salt solid used in equilibrium calculation is MgCl₂·6H₂O.^c Pitzer interaction parameters for K⁺ and NO₃⁻ pair are only available at 25°C.

The resulting percent differences between relative humidity values from EQ3/6 calculation predictions and experimental data for the salt deliquescence ranges from less than a percent to approximately 14.3 percent (Table 7.4-2). The highest values for percent differences are largely restricted to the MgCl₂ salt when compared to the other salts. But this difference is less than 5 percent in relative humidity, and the IDPS model indicates that below 40 percent RH it has a general uncertainty of 15 percent (Table 6.12-1). Therefore, this quantity of uncertainty is well within the expected range.

For mixed electrolytes, the maximum percent difference is approximately 10.1 percent (approximately 5 percent RH). In this mid-RH range, the IDPS model is determined to have an uncertainty of 10 percent RH (Table 6.12-1), affirming the applicability of the Pitzer model in modeling mixed salts. Though for the mixed salt case, NaCl + NaNO₃ + KNO₃, the Pitzer parameter for KNO₃ is only available at 25°C.

Overall, the differences between predicted and experimental values are less than the IDPS modeling uncertainty. In addition, these results easily fall within the plus or minus 10 percent RH validation objective of the IDPS model (BSC 2004 [DIRS 169863], Section 7.5.3). Therefore, the present comparisons between two different sets of experimental data and code

predictions confirm the validity in the application of the computational method to predict salt deliquescence points at an acceptable level of accuracy.

7.5 VALIDATION SUMMARY

The three models (for gas, seepage and dust) in this report have been validated by applying the acceptance criteria based on an evaluation of the model's relative importance to the potential performance of the repository system. All validation requirements defined in the technical work plan (BSC 2004 [DIRS 171156], Sections 2.2.2.2 and 2.2.2.4) have been fulfilled. These include comparison of the abstraction model results to the results of the validated model (Section 7.2.2), corroboration of model results with additional laboratory results (Section 7.2.3), corroboration with alternative conceptual models (Section 6.11), and corroboration with information published in referred journals (Sections 7.3 and 7.4 for evaporation and deliquescence, respectively). Activity requirements for confidence building during model development have also been satisfied. The model development activities and postdevelopment validation activities described establish the scientific bases for the physical and chemical environment models. Based on this, the physical and chemical environment models used in this report are considered to be sufficiently accurate and adequate for their intended purpose and to the level of confidence required by the model's relative importance to the potential performance of the repository system.

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8. CONCLUSIONS

8.1 SUMMARY AND MODEL FINDINGS

The EBS chemical environment abstractions provide a quantitative description of the pH, ionic strength (I), and major ionic and elemental compositions of waters in contact with the waste package, drip shield, and the invert. Brines that form by evaporative concentration of the crown seepage can potentially affect corrosion on the waste package and drip shield, and influence radionuclide mobility in the invert. Compositional parameters in the waters contacting the drip shield and waste package, such as pH, or the ratio of chloride to nitrate are important in assessing potential localized corrosion (BSC 2004 [DIRS 169984], Section 6.4.4; BSC 2004 [DIRS 169845]). Acidic or alkaline pH values in the water of the invert may affect the solubility of radionuclides. Changes ionic strength of the water in the invert may reduce the mobility of colloidal particles transporting sorbed radionuclides.

Potential water compositions of crown seepage from the thermal-hydrological-chemical (THC) seepage model are abstracted into 11 possible waters that represent different brine types upon evaporation (Section 6.6). These abstracted waters are used to generate a set of 198 lookup tables to represent evaporated crown seepage and invert waters for TSPA-LA. The lookup tables represent a response surface for each bin covering a range of temperatures (100°C to 40°C), $p\text{CO}_2$ (10^{-4} to 10^{-2} bars) and relative humidity. The generation of these tables is discussed in Section 6.9. The total range in chemistry of the crown seepage and invert waters (e.g., pH, I, Cl, NO_3/Cl), as predicted by the lookup tables, is discussed in Section 6.13.

The EBS P&CE seepage evaporation abstraction shows that corrosive calcium and magnesium chloride brines are unlikely to form on waste packages and drip shields (Tables 6.13-1 and 6.13-8), and, if they do form, persist for only very short times soon after closure of the repository. The most likely brines to form are sodium chloride- or sodium carbonate-type brines (Table 6.13-8, Bins 7 through 11), which are far less aggressive with respect to corrosion of engineered barrier materials. $\text{Cl}:\text{NO}_3$ ratios for all bins expected to contact drip shields and waste packages are shown in Figure 6.13-29. The mineral assemblages that precipitate during evaporation of the brines in the 99 crown seepage evaporative lookup tables are reported in Table 6.13-6.

Lookup tables that represent both seepage water and invert water have been provided with instructions (Section 6.15) on how to select the appropriate chemical values from the lookup tables. These lookup tables can be used as source chemistry for waters fluxing into the invert.

Stainless steel ground support and low-alloy or carbon steel committed materials have their chemical composition and corrosion rates compiled in Section 6.4. The short-lived materials, such as low-alloy or carbon steel, corrode rapidly in the high humidity environment of the drift and do not affect crown seepage water as they are located in the invert. Oxygen gas fugacity of the in-drift atmosphere is determined to be sufficient to maintain an oxidative environment during the corrosion of the low-alloy or carbon steels (Section 6.7).

The Stainless Steel Type 316L corrosion rate output allows for determination of ground support interactions with seepage. This material comprises the perforated sheet ground support component that spans the crown of the drift, when required. Abstracted modeling and sensitivity

studies of crown seepage interacting with Stainless Steel Type 316L as calculated in Section 6.8.4, indicate that the effects of the active corrosion of Stainless Steel Type 316L are insignificant near 100 and 98 percent relative humidity. Based on these results and the results of the uncertainty calculations presented in Section 6.12.4.1, it is reasonable to conclude that the active corrosion of ground support will not significantly influence the composition of the seepage at any time.

Dust that settles onto the waste package and drip shield from natural sources and repository construction processes could affect repository performance with respect to corrosion. During and for a while after the heat pulse, when temperatures are above 100°C, no liquid water is expected to flow in the drift (Section 6.2). Thus, the only waters that are likely to be present are those formed by deliquescence of the salt within dust. Most of the dust is derived from the volcanic tuff host rock and most brines that form by dust deliquescence are not aggressive with respect to corrosion of titanium or Alloy 22. The potential for corrosive brines to form is very low and if they do form they will not persist long (Section 6.13).

To quantitatively investigate the effect of deliquescent brines, measured compositions of dust leachate water are abstracted into 6 possible waters that represent dust leachate compositions upon evaporation (Section 6.10). These abstracted waters are used to generate a set of 90 lookup tables to represent deliquescence in dust. The lookup tables represent a response surface for each bin covering a range of temperatures (140°C to 40°C), $p\text{CO}_2$ (10^{-4} to 10^{-2} bars) and relative humidity. The total range of dust leachate chemistry (e.g., pH, I, Cl, NO_3/Cl) covered in the generation of the lookup tables is discussed in Section 6.13. Minerals that precipitate in each of the 6 dust leachate bins during the course of evaporation are reported in Table 6.13-7.

8.2 SUMMARY OF MODEL ABSTRACTION FOR TOTAL SYSTEM PERFORMANCE ASSESSMENT

8.2.1 Summary of the Total System Performance Assessment Lookup Tables

Foldout F/O 8.2-1 summarizes the recommended usage of the lookup tables developed in Sections 6.6, 6.7, 6.9, and 6.10 for use on the engineered barrier surface. The instructions and restrictions for use of the scenarios depicted by this foldout are summarized in Sections 6.13 and 6.15. The foldout describes the use of this model by the TSPA to determine water chemistries during active seepage and deliquescence of dust on the waste packages and drip shields. Section 6.15.2 gives the instructions for implementing lookup tables to determine chemistry in the invert. Section 8.2.2 lists the lookup table data tracking numbers (DTNs).

During preliminary implementation of the seepage lookup tables in the TSPA, it was discovered that the GoldSim software (BSC 2003 [DIRS 161572]) can't handle duplicated values for the independent parameter in the tables. This occurs in the lookup tables when mineral precipitation occurs, at which point the exact same activity of water (the independent parameter) is duplicated to include the new mineral. In order to provide a set of lookup tables to the TSPA that could be utilized, the lookup tables in output DTN: MO0304SPACSALT.000 were modified; in cases where the independent parameter (RH) was repeated, one of the values was modified slightly to eliminate the duplication without removing chemical parameter values from the dataset. The modified versions of the files in the DTN: MO0304SPACSALT.000 are found in a new output

DTN: MO0310SPAPCEGS.000; modifications are indicated in the lookup table by red text. All other users of data from this report should use the original files archived in DTN: MO0304SPACSALT.000.

8.2.2 Data Tracking Numbers for Data Generated in This Report

Tables 8.2-1 and 8.2-2 list the DTNs for data generated in this report. Table 8.2-1 is for data generated to feed the TSPA-LA and Table 8.2-2 is for supporting data used in development of the TSPA-LA data feeds. These data are also summarized in Appendix A.

Table 8.2-1. EBS Physical and Chemical Environment Model Output DTNs Derived for use in the Total System Performance Assessment-License Application Model

Data Tracking Number	Location In Text	Description of TSPA Parameters
MO0310SPAEBSCB.003	Tables 6.6-3 to 6.6-14 Sections 6.6.4 to 6.6.6 Sections 6.6.7.1 and 6.6.7.2 Section 6.11.1.1 Section 6.12.3.1 Section 6.15.1.1 Section 6.15.2 Section 7.2.1	Bin history maps for each of the 5 starting THC waters for both crown seepage and invert wicking
MO0308SPACO2GL.001	Tables 6.7-1 to 6.7-5 Sections 6.7.2.1 and 6.7.2.2 Section 6.12.5.3 Section 6.13.2.1 Section 6.15.1.1 Section 6.15.2	$p\text{CO}_2$ time-history lookup tables for each of the 5 starting THC waters for both crown seepage and invert wicking
MO0310SPAPCEGS.000 These values are for TSPA Goldsim software implementation. All other users should use the lookup tables archived in MO0304SPACSALT.000	Tables 6.9-6 and 6.9-7 Sections 6.9.3 and 6.9.4 Section 6.11.2 Section 6.12.5 Sections 6.12.5.2 and 6.12.5.3 Section 6.15.1.1 Section 6.15.2 Section 7.2.1 Section 8.2.1	198 THC seepage lookup tables containing pH, I, Cl, F, N, and other ions as a function of drift relative humidity, associated with the 11 abstraction bins, three starting temperatures (100°C, 70°C, and 40°C) and three $p\text{CO}_2$ values (10^{-4} , 10^{-3} and 10^{-2} bars) – in all 99 tables for evaporation and 99 tables for condensation. Also included is a relative humidity map to interface between the evaporation lookup tables and the condensation lookup tables.
MO0310SPADLALT.001	Table 6.10-14 Section 6.10.6.5 Section 6.10.8 Section 6.12.5 Section 6.12.5.2 and 6.12.5.3 Section 6.15.1.2	54 dust leachate lookup tables containing pH, I, Cl, F, N, Cl/N ratio, and other ions as a function of relative humidity, associated with the 6 abstraction bins, three starting temperatures (100°C, 70°C, and 40°C) and three $p\text{CO}_2$ values (10^{-4} , 10^{-3} and 10^{-2} bars).
MO0310SPADLHTL.000	Table 6.10-14 Section 6.10.6.5 Section 6.12.5 Section 6.12.5.2 and 6.12.5.3 Section 6.15.1.2	36 dust leachate lookup tables containing pH, I, Cl, F, N, Cl/N ratio, and other ions as a function of relative humidity, associated with the 6 abstraction bins, two starting temperatures (120°C, 140°C) and three $p\text{CO}_2$ values (10^{-4} , 10^{-3} and 10^{-2} bars).

Table 8.2-1. EBS Physical and Chemical Environment Model Output DTNs Derived for use in the Total System Performance Assessment-License Application Model (Continued)

Data Tracking Number	Location In Text	Description of TSPA Parameters
MO0310SPADLBU4.001	Table 6.7-7 Tables 6.10-4 to 6.10-10 Table 6.12-5 Section 6.7.5 Section 6.10.4 Sections 6.10.5.2 and 6.10.5.3 Section 6.10.5.5 Section 7.2.4	Percentage of waters in each of the 6 dust leachate bins
MO0311SPAEPMUT.000	Tables 6.12-4 and 6.12-8, Tables 6.12-29 and 6.12-30	Uncertainty values for pH, ionic strength, Cl, and Cl-NO ₃ parameters
SN0403T0503404.001	Section 4.1.5 Section 6.11.2	Maximum relative humidity (RH) of halite precipitation extracted from P&CE seepage evaporation lookup tables

EBS Environment Water Chemistry Derivations by Source and Location for TSPA:

I. Crown Seepage and Dust Leachate Effects on Waste Package and Drip Shield

Figure 8.2-1. EBS Environment Water Chemistry Derivations for Total System Performance Assessment/License Application on the Waste Package and Drip Shield (P/Q)

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Table 8.2-2. EBS Physical and Chemical Environment Model Supplemental Output DTNs

Output DTN	Location In Text	Title
SN0310T0510102.010	Tables 6.10-2 and 6.10-3 Table 6.10-11 Table 6.12-5 Table 6.12-9 Sections 6.10.2 to 6.10.4 Sections 6.10.5.1 and 6.10.5.2 Section 6.10.5.5 Section 6.10.6.1 Section 6.10.8 Section 7.2.4	Analysis of In-Drift Dust Leachates at 25 °C to Various Evaporation Relative Humidity (RH) Levels
MO0304SPAA11GC.000	Tables 6.7-6 Tables 6.9-1 and 6.9-2 Section 6.9.1	EBS THC Seepage Abstraction 11 Bin EQ3 3o File Water and Gas Chemistry Extraction
SN0310T0510102.011	Tables 6.10-12 and 6.10-13 Table 6.12-9 Section 6.10.6 Sections 6.10.6.2 and 6.10.6.3	Dust Leachate Abstraction TSPA-LA Lookup Table Eq3/6 Input and Output Files, Low Temperature
SN0310T0510102.012	Tables 6.10-12 and 6.10-13 Section 6.10.6 Sections 6.10.6.2 and 6.10.6.3	Dust Leachate Abstraction TSPA-LA Lookup Table Eq3/6 Input and Output Files, High Temperature
MO0304MWDSAB11.001	Tables 6.9-3 and 6.9-4 Table 6.12-9 Section 6.8.2 Section 6.8.4.1 Section 6.9.1 Section 6.12.4.1.3	EBS THC Seepage Abstraction 11 Bin EQ3 3i, 3p, and 3o Files
MO0304SPACSALT.000 These values are for users other than TSPA Goldsim software implementation. For TSPA implementation use lookup tables archived in MO0310SPAPCEGS.000	Table 6.9-6 Table 6.9-7 Section 6.9.3 Section 6.12.5 Section 6.12.5.3 Section 6.15.1.1 Section 6.15.2 Table 8.2-1	198 THC seepage lookup tables containing pH, I, Cl, F, N, and other ions as a function of drift relative humidity, associated with the 11 abstraction bins, three starting temperatures (100°C, 70°C, and 40°C) and three $p\text{CO}_2$ values (10^{-4} , 10^{-3} and 10^{-2} bars) – in all 99 tables for evaporation and 99 tables for condensation. Also included is a relative humidity map to interface between the evaporation lookup tables and the condensation lookup tables.
MO0303MWDSCMAB.000	Table 6.6-1 Section 6.6.3 Section 6.7.3 Section 6.9.1	THC Seepage Chemistry Model Abstraction Binning EQ3 Input, Pickup and Output Files
MO0303MWDEBSSM.000	Table 6.6-1 Tables 6.6-13 and 6.6-14 Sections 6.6.3 and 6.6.4 Section 6.7.3	EBS Abstraction of the THC Seepage Model: Binning Analysis Evaporation to 65% RH EQ6 Input and Output Files
MO0310SPAEBSSUE.002	Section 6.12.3.1 Section 7.2.1	EBS Chemistry Unevaporated Binning Abstraction Statistics
MO0304MWDEBSSA.000	Table 6.9-5 Table 6.12-9 Section 6.9.2 Section 7.2.2	EBS THC Seepage Abstraction TSPA-LA Lookup Table EQ6 Input and Output Files

Table 8.2-2. EBS Physical and Chemical Environment Model Supplemental Output DTNs (Continued)

Output DTN	Location In Text	Title
MO0407SPAPCEML.005	Table 4.1-2 Tables 6.4-11, 6.4-15, and 6.4-18 Section 4.1.1	EBS P&CE Model Longevity of Materials Evaluation
MO0310SPAPCEUA.002	Tables 6.12-21 to 6.12-28 Sections 6.12.4.2.3 and 6.12.4.2.4 Sections 6.12.4.3.2 and 6.12.4.3.3 Section 6.12.4.4 Sections 6.12.4.4.1 and 6.12.4.4.2	EBS P&CE Uncertainty Analyses for $p\text{CO}_2$, Br, and MineralSuppressions
SN0303T0510102.004	Tables 7.4-1 and 7.4-2	EQ3/6 (Version 8.0) Input/Output Data Files – Salt Deliquescence Point Modeling as A Function of Temperature
MO0310SPAPCEAC.002	Tables 6.11-1 to 6.11-14 Section 6.11.1.1	EBS P&CE Alternate Conceptual Model Calculations
SN0312T0510102.013	Tables 4.1-23 and 4.1-24 Tables 6.8-2 and 6.8-5 Tables 6.12-10 to 6.12-19 Sections 6.8.2 and 6.8.3 Sections 6.8.4.1 and 6.8.4.3 Section 6.12.4.1	EBS P&CE Model Stainless Steel Abstraction
MO0310SPAPCELA.002	Tables 6.13-7 and 6.13-9 Section 6.12.4.2.4 Sections 6.13.2.1 to 6.13.2.3 Section 6.13.4.2	EBS P&CE Model Dust Leachate Analyses Spreadsheets and Data
MO0312SPAPCESA.002	Tables 6.13-1, 6.13-2, 6.13-6, and 6.13-8 Section 6.13 Sections 6.13.1.3, 6.13.4.1, and 6.13.5.2 Section 7.2.1	EBS P&CE Model THC Seepage Analysis Spreadsheets
MO0304SPACPSLT.000	Section 6.13.1.2	Combined In-Drift Precipitates/Salts Model Lookup Table for Seepage Evaporation Abstractions for All Bins
MO0310SPAEBSSB.002	Section 6.12.3.1	EBS P&CE Model THC Seepage Bin Uncertainty Analyses
MO0310SPAPCELT.000	Tables 6.12-2 and 6.12-6 Section 6.12.3.1	EBS P&CE Log Transform Of Uncertainty Data
MO0311SPASADLS.000	Section 6.10.8	EBS P&CE Sensitivity Analyses On Dust Leachate Silica Values
MO0406MWDARHPW.000	Section 7.2.3 Table 7.2-1	Abstraction of Repository Horizon Porewaters using EQ3/6.
SN0404T0510102.014	Section 7.3	EBS P&CE Model, Sierra Nevada Spring Water Validation; EQ3/6 Runs and Results
SN0406T0510102.015	Section 7.2.2	EBS P&CE Model Validation Interpolation Calculations
SN0407T0510102.017	Table 4.1-17 Sections 4.1.2 and 4.1.3 Sections 6.7.1.1 to 6.7.1.3	In-Drift Gas Flux And Oxygen Demand

8.3 MODEL UNCERTAINTY AND RESTRICTIONS

Uncertainties in the output from the EBS physical and chemical environment (P&CE) model are summarized in this section. Direct inputs to the model are tabulated and discussed in Section 4.1, but the uncertainties associated with those inputs are discussed in the subsections of Section 6 where they are used. The effects of input uncertainties are discussed in more detail in Section 6.12. Limitations and constraints on the use of the model and its outputs are discussed in Section 6.13 with the discussions of the various components and features of the overall EBS P&CE model. Specific limitations involved in the model are listed in Section 1.3.

The EBS P&CE model uses five primary inputs, and each has uncertainty associated with it. These inputs are:

- Composition of water entering the drift
- Composition of dust predicted to settle on repository surfaces
- *In-Drift Precipitates/Salts (IDPS) Model* (BSC 2004 [DIRS 169863]) and its associated data bases (thermodynamic data and other technical information not specific to the site used in the geochemical modeling that results in the model output)
- Composition and flux of in-drift gases
- Amounts and characteristics of engineered materials to be placed in the drift (ground support, emplacement rails, etc.).

For evaluating repository performance, five parameters have been identified as output from this model that will be used as direct input to TSPA calculations: 1) chloride ion concentration, 2) chloride/nitrate molar ratio, 3) ionic strength, 4) pH, and 5) relative humidity point at which salt minerals deliquesce and an aqueous phase appears.

As explained in Section 6.12, of the five inputs, only three were found to have uncertainties that would propagate into the output parameters that feed the TSPA: 1) the IDPS model, 2) the abstracted incoming seepage waters, and 3) aqueous solutions that could result from deliquescence of salts in dust.

An evaluation of the IDPS model was conducted to determine its contribution to error in predicting the parameters of interest as explained in Section 6.12.2. A statistical evaluation of the TSPA parameter feeds (except relative humidity, which was not relevant to this evaluation) in the 11 bins of seepage water and the 6 bins for dust deliquescence water was conducted as explained in Section 6.12.3. This evaluation demonstrated that there is a sufficiently large variability within the bins to warrant the creation of a discretization error band around the median water's values for parameters that need be propagated by the TSPA process.

Uncertainties from these sources are propagated in a realistic and representative way to TSPA. There the model and abstraction uncertainty are directly combined to generate total error bands for the parameters of interest to TSPA. Appropriate distribution for the error ranges was selected, and instructions for how to implement the errors were developed in Section 6.12.5.

8.4 YUCCA MOUNTAIN REVIEW PLAN CRITERIA ASSESSMENT

This model report predicts results that directly pertain to the abstraction of the quantity and chemistry of water contacting engineered barriers and waste forms. This section summarizes the contents of this report as they apply to NRC criteria for a detailed review of that abstraction.

8.4.1 Quantity and Chemistry of Water Contacting Engineered Barriers and Waste Forms—Acceptance Criteria

These criterion are from *Yucca Mountain Review Plan, Final Report* (NRC 2003 [DIRS 163274], Section 2.2.1.3.3.3, which is from 10 CFR 63.114(a)–(c) and (e)–(g) [DIRS 156605]).

8.4.1.1 Acceptance Criterion 1—System Description and Model Integration are Adequate

(1) TSPA adequately incorporates important design features, physical phenomena, and couplings, and uses consistent and appropriate assumptions throughout the quantity and chemistry of water contacting engineered barriers and waste forms abstraction process;

The effects of coupled processes (Section 6.3) have been considered in part in the development of this model. For example, THC effects on input water compositions are incorporated in the THC model output (Section 4.1.3) used as input to the P&CE model. Thermal-hydrological-chemical processes are at the heart of the in-drift water chemistry evolution presented in this report. The analyses presented in this report use current design information (Sections 4.1 and 6.4), and are based on physical phenomena expected within repository drifts (Section 6.2). Coupled processes that were considered and screened out from further consideration in this report and their rationale for exclusion, are presented in *Engineered Barrier System Features, Events, And Processes* (BSC 2004 [DIRS 169898], Section 6.2.60). Assumptions (Section 5) contained in this report are appropriate and are consistent with similar assumptions in related documents. These factors are included in the analyses leading to the output parameters (Section 6.13), which may be used to assess engineered barrier and waste form degradation.

(2) The abstraction of the quantity and chemistry of water contacting engineered barriers and waste forms uses assumptions, technical bases, data, and models that are appropriate and consistent with other related DOE abstractions. For example, the assumptions used for the quantity and chemistry of water contacting engineered barriers and waste forms are consistent with the abstractions of “Degradation of Engineered Barriers” (Section 2.2.1.3.1); “Mechanical Disruption of Engineered Barriers” (Section 2.2.1.3.2); “Radionuclide Release Rates and Solubility Limits” (Section 2.2.1.3.4); “Climate and Infiltration” (Section 2.2.1.3.5); and “Flow Paths in the Unsaturated Zone” (Section 2.2.1.3.6). The descriptions and technical bases provide transparent and traceable support for the abstraction of quantity and chemistry of water contacting engineered barriers and waste forms;

This report uses the same technical bases and other information as are used in other LA-supporting documents concerned with engineered barrier and waste form performance. The conceptual model that forms the basis for this report (Section 6.2) and its assumptions (Section 5) are consistent with other engineered system models and repository design. Primary input (Section 4.1) is taken from the UZ THC model to develop both the in-drift water and gas chemistries. The IDPS model is used in conjunction with the THC model output to generate in-drift water chemistry. Section 6.2 provides details of these model interfaces. Input water fluxes are dealt with in *Seepage Model for PA Including Drift Collapse* (BSC 2003 [DIRS 167652]). The descriptions and technical bases are recorded to provide inherently transparent and traceable support for the abstraction of in-drift water chemistry.

(3) *Important design features, such as waste package design and material selection, backfill, drip shield, ground support, thermal loading strategy, and degradation processes, are adequate to determine the initial and boundary conditions for calculations of the quantity and chemistry of water contacting engineered barriers and waste forms;*

Initial and boundary conditions for this model are based on descriptions of design features (Section 6.4) and predicted behavior of the EBS (Section 6.2) as documented in Project design documents and in other barrier-specific models and abstractions. This model includes consideration of the chemical effects of corrosion on engineered materials (Sections 6.7 and 6.8).

(4) *Spatial and temporal abstractions appropriately address physical couplings (thermal-hydrologic-mechanical-chemical). For example, the DOE evaluates the potential for focusing of water flow into drifts, caused by coupled thermal-hydrologic-mechanical-chemical processes;*

The abstractions in the P&CE model incorporate the effects of a number of different coupled processes in its evaluation of in-drift water chemistry. For example, THC physical couplings are included implicitly through the THC model output as well as through the temporal abstraction methodology. Another example is the analysis addressing the impact of corrosion of ground support materials impact. This analysis takes into account various thermal-hydrological-mechanical-chemical effects, as do the corrosion rates used in the analysis. Coupled processes formally classified as FEPs are discussed briefly in Section 6.14 and documented in more detail in various FEPs reports such as *Engineered Barrier System Features, Events, And Processes* (BSC 2004 [DIRS 169898], Section 6.2.60). These reports contain straightforward screening arguments if the FEP is excluded from further consideration and a description of the TSPA disposition if it is included. The master list of FEPs is contained in DTN: MO0407SEPFELA.000 [DIRS 170760].

(5) *Sufficient technical bases and justification are provided for total system performance assessment assumptions and approximations for modeling coupled thermal-hydrological-mechanical-chemical effects on seepage and flow, the waste package chemical environment, and the chemical environment for radionuclide release. The effects of distribution of flow on the amount of water contacting the engineered barriers and waste forms are consistently addressed, in all relevant abstractions;*

Assumptions (Section 5) and approximations pertaining to coupled processes in the P&CE model as well as their technical bases and justification are provided throughout the report. FEPs involving coupled processes are discussed with their technical bases in Section 6.14. The seepage abstraction is consistent with the THC seepage model and the lookup tables are designed to couple the thermal hydrology of the drift with the chemical environment in drift. This model report is not concerned with distribution of flow within the drift.

- (6) The expected ranges of environmental conditions within the waste package emplacement drifts, inside of breached waste packages, and contacting the waste forms and their evolution with time are identified. These ranges may be developed to include:
  - (i) Effects of the drip shield and backfill on the quantity and chemistry of water (e.g., the potential for condensate formation and dripping from the underside of the shield)
  - (ii) Conditions that promote corrosion of engineered barriers and degradation of waste forms;
  - (iii) Irregular wet and dry cycles;
  - (iv) Gamma-radiolysis; and
  - (v) Size and distribution of penetrations of engineered barriers;

This report develops and presents the expected ranges of environmental conditions within the drifts (Section 6.7, 6.9, and 6.10). Although this model does characterize conditions that affect corrosion of engineered barriers (Section 6.13), it does not consider the effect of the drip shield or backfill (current design does not include backfill) on the quantity and chemistry of water. Wet and dry cycles, gamma radiolysis, and size and distribution of engineered barriers are not the subject of this report, although information from it may be used to assess those factors.

- (7) The model abstraction for quantity and chemistry of water contacting engineered barriers and waste forms is consistent with the detailed information on engineered barrier design and other engineered features. For example, consistency is demonstrated for:
  - (i) Dimensionality of the abstractions;
  - (ii) Various design features and site characteristics; and
  - (iii) Alternative conceptual approaches.

Analyses are adequate to demonstrate that no deleterious effects are caused by design or site features that the DOE does not take into account in this abstraction;

The chemistry of water contacting engineered barriers was developed using detailed information on various designed (engineered) features and site characteristics (Section 4.1), although this

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 169856], 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 169984], Sections 6.3.1 and 6.3.2), to determine if localized corrosion is occurring on the waste packages.

(12) Guidance in NUREG-1297 (Altman et al. 1988 [DIRS 103597]) and NUREG-1298 (Altman et al. 1988 [DIRS 103750]), or other acceptable approaches, is followed.

Inputs were selected and documented according to applicable BSC procedures, which comply with NUREG-1297 and -1298 (Section 4.1).

8.4.1.2 Acceptance Criterion 2—Data are Sufficient for Model Justification

(1) Geological, hydrological, and geochemical values used in the license application are adequately justified. Adequate description of how the data were used, interpreted, and appropriately synthesized into the parameters is provided;

The selection and justification of geological, hydrological, and geochemical values for use and sources of input data are contained in Section 4.1 and tabulated in the DIRS. Further details of model development as related to the use, interpretation, and synthesis of data into parameters are presented throughout Section 6, especially in Section 6.6. The model was developed using water chemistry and dust data collected in the ESF and adjoining facilities. The geochemical analyses presented in this report are based on a chemical thermodynamic database developed for this use from internationally accepted thermodynamic data (Sections 6.2 and 6.5).

(2) Sufficient data were collected on the characteristics of the natural system and engineered materials to establish initial and boundary conditions for conceptual models of thermal-hydrological-mechanical-chemical coupled processes, that affect seepage and flow and the engineered barrier chemical environment;

Data and technical information collected from field and experimental sources, and from literature searches for this model are discussed for engineered materials in Section 4.1 (engineered components) and Section 6.4 (design features), and for natural system characteristics in Section 6.5 (mineralogical information) and in Section 6.6 (THC model). Natural system data are used to develop the THC model, which is a major input to this model (Section 6.6). The natural system data are used to establish initial and boundary conditions that affect seepage and flow and are discussed in Section 6.6. The discussion of the initial and boundary conditions that affect seepage and flow for the engineered material data is discussed in Section 6.8. The effects on the chemical environment in the waste package from collected data are discussed in *In-Package Chemistry Abstraction* (BSC 2004 [DIRS 167621]).

(4) Sufficient information to formulate the conceptual approach(es) for analyzing water contact with the drip shield, engineered barriers, and waste forms is provided;

The conceptual approaches of this report's modeling of seepage and dust deliquescence waters are supported. This support comes both from other model reports (e.g., IDPS and THC, Section 6.2) as well as the analyses presented within this report such as: mineral inclusion or suppression

(Section 6.5.5), oxygen availability (Section 6.7), and crown seepage interaction with the stainless steel ground support (Section 6.8).

8.4.1.3 Acceptance Criterion 3—Data Uncertainty Is Characterized and Propagated Through the Model Abstraction

(1) Models use parameter values, assumed ranges, probability distributions, and bounding assumptions that are technically defensible, reasonably account for uncertainties and variabilities, and do not result in an under-representation of the risk estimate;

The model parameter values were selected based on the characteristics of the input and are considered representative of the natural and engineered systems (Sections 4.1, 6.4, 6.5, 6.6, and 6.10). Ranges, probability distributions, and bounding assumptions were considered in assessing boundary conditions and input uncertainties and variabilities, which were propagated through the model as described in Section 6.12. Further propagation through TSPA-LA implementation is described in Section 6.15. When modeling decisions were necessary, the choices were made to result in conservative outcomes that avoid dilution of overall risk (Sections 6.9, 6.10, and 6.12).

(2) Parameter values, assumed ranges, probability distributions, and bounding assumptions used in the total system performance assessment calculations of quantity and chemistry of water contacting engineered barriers and waste forms are technically defensible and reasonable, based on data from the Yucca Mountain region (e.g., results from large block and drift-scale heater and niche tests), and a combination of techniques that may include laboratory experiments, field measurements, natural analog research, and process-level modeling studies;

The parameter values, assumed ranges, probability distributions, and bounding assumptions developed by other models based on site-specific data are discussed in Sections 6.6 and 6.11. Values, ranges, and distributions obtained from other techniques mentioned above include such information as the thermodynamic databases, discussed in Section 4.1.4 with additional discussion in *In-Drift Precipitates/Salts Model* (BSC 2004 [DIRS 169863]); corrosion data, discussed in Sections 6.4 and 6.8; and mineralogy data discussed in Appendix D. Much of the data founding model development was collected in the ESF and adjoining facilities. This included seepage water samples and dust samples. Environmental conditions imposed on model development (temperatures, RH, and moisture contents) were consistent with data collected from the drift scale test and other related tests. The validation for the THC seepage abstraction has been performed against results from the THC seepage model, which was validated against data from the drift scale test. Other laboratory and natural analog information was used for validation of portions of the model (Section 7).

(3) Input values used in the total system performance assessment calculations of quantity and chemistry of water contacting engineered barriers (e.g., drip shield and waste package) are consistent with the initial and boundary conditions and the assumptions of the conceptual models and design concepts for the Yucca

Mountain site. Correlations between input values are appropriately established in the U.S. Department of Energy total system performance assessment. Parameters used to define initial conditions, boundary conditions, and computational domain in sensitivity analyses involving coupled thermal-hydrological-mechanical-chemical effects on seepage and flow, the waste package chemical environment, and the chemical environment for radionuclide release, are consistent with available data. Reasonable or conservative ranges of parameters or functional relations are established;

The input values (Section 4.1) were developed using initial and boundary conditions and assumptions (Section 5) common to other conceptual models and compatible with design concepts. Sensitivity studies involving coupled effects on the chemical environment were conducted (e.g., Section 6.12). The initial and boundary conditions and computational domain for these sensitivity analyses were determined using parameters that are consistent with available data. This report uses the same technical bases and other information as are used in other LA-supporting documents concerned with engineered barrier and waste form performance. The conceptual model that forms the basis for this report is consistent with other engineered system models and repository design. Primary input is taken from the UZ THC model and the IDPS model is used to generate in-drift water chemistry. Sections 6.2 and 6.6 provide details of these model interfaces.

Correlations between input values were established and used at various points in the P&CE model (Sections 6.6, 6.7, and 6.13). For example, the THC input water and gas chemistries through time are correlated to each other, to temperature, and to relative humidity. Additionally, the correlation of chloride and nitrate are accounted for in the way their uncertainties are determined (Section 6.12.3.1) and implemented (Section 6.12.5.3).

The ranges of parameters and functional relations developed in this report, primarily as lookup tables (Section 6.13), are considered reasonable or conservative. Section 6.15 discusses the appropriate use of these tables, which are response surfaces that relate water chemistry to relative humidity, temperature, $p\text{CO}_2$, and time.

(4) Adequate representation of uncertainties in the characteristics of the natural system and engineered materials is provided in parameter development for conceptual models, process-level models, and alternative conceptual models. The U.S. Department of Energy may constrain these uncertainties using sensitivity analyses or conservative limits. For example, the U.S. Department of Energy demonstrates how parameters used to describe flow through the EBS bound the effects of backfill and excavation-induced changes;

Uncertainties in natural system characteristics are included in the THC model output, which is used as direct input to this model. Uncertainties in the Pitzer (natural system) and the *data0.ymp.R2* (engineered systems) thermodynamic databases used as direct input to this model are discussed in Section 6.12, with additional mineralogy discussion in Appendix D. Engineered materials uncertainties are specifically considered in Section 6.12, with further extensive discussions on the effects of dust in Section 6.10. Those uncertainties are evaluated using

sensitivity analyses as discussed in Sections 4.1.8 and 6.12. Section 6.12 discusses five key uncertainties including engineered materials and natural systems parameters.

8.4.1.4 Acceptance Criterion 4—Model Uncertainty Is Characterized and Propagated Through the Model Abstraction

(1) Alternative modeling approaches of features, events, and processes are considered and are consistent with available data and current scientific understanding, and the results and limitations are appropriately considered in the abstraction;

The evaluation of FEPs documented in Section 6.14 is based on the model results developed in this report, including the alternative modeling discussed in Section 6.11. This alternative modeling is consistent with available data and scientific understanding. The results and limitations of the alternative FEP modeling and their impact on the engineered barrier chemical environment are presented in Section 6.14.

(2) Alternative modeling approaches are considered and the selected modeling approach is consistent with available data and current scientific understanding. A description that includes a discussion of alternative modeling approaches not considered in the final analysis and the limitations and uncertainties of the chosen model is provided;

Section 6.11 describes several alternative modeling approaches considered for various P&CE submodels. One submodel, the in-drift gas abstraction, was deemed to not need an explicit alternative model (also see Section 6.11 for this screening rationale). None of the alternative models were selected for further use. For all model alternatives brief descriptions and the rationale for exclusion are included as well as references to other reports and sections within this report for further detail. These references also contain information about the models that were selected including their technical bases, limitations, and uncertainties.

Section 6.11 also provides an extensive investigation of a single model involving an alternative method for clustering waters during the abstraction of THC seepage waters. The exclusion rationale is based upon a comparison of results from the alternative model with those from the selected approach (Section 6.6). The selected approach is consistent with available data and current scientific understanding. The uncertainties and limitations of various selected approaches are discussed throughout the report (Sections 1.3, 6.6, 6.12, and 8.3).

(3) Consideration of conceptual model uncertainty is consistent with available site characterization data, laboratory experiments, field measurements, natural analog information and process-level modeling studies; and the treatment of conceptual model uncertainty does not result in an under-representation of the risk estimate;

Uncertainties in inputs and in analytical methodology are considered in the development of the conceptual model (Section 6.2) and output parameters (Section 6.15). Discussion of uncertainty in the conceptual model appears in various places throughout the report. One example is Section 6.12.1, where quotations from *Drift-Scale THC Seepage Model* (BSC 2004

[DIRS 169856], 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*

same assumptions and approximations demonstrated to be appropriate for process-level models or closely analogous natural or experimental systems. For example, abstractions of processes, such as thermally induced changes in hydrological properties, or estimated diversion of percolation away from the drifts, are adequately justified by comparison to results of process-level modeling, that are consistent with direct observations and field studies;

The abstracted model is based on the same assumptions and approximations demonstrated to be appropriate for process-level models. Coupled thermal-hydrological-chemical considerations are the dominant factor in the development of this model abstraction. The output of this model is a tabulation of chemical conditions as a function of physical environmental conditions that is consistent with process-level modeling as demonstrated by model validation results (Section 7), which are in turn consistent with direct observations from laboratory and field studies.

(3) Accepted and well-documented procedures are used to construct and test the numerical models that simulate coupled thermal-hydrological-mechanical-chemical effects on seepage and flow, engineered barrier chemical environment, and the chemical environment for radionuclide release. Analytical and numerical models are appropriately supported. Abstracted model results are compared with different mathematical models, to judge robustness of results.

Accepted and well-documented procedures contained in the quality assurance program (Section 2) governed the development of this report and the work it documents. The PC&E model was constructed, supported, and documented according to AP-SIII.10Q. Test and validation methods (Section 7), including comparison of abstracted output with that of other relevant models, also comply with AP-SIII.10Q as well as with applicable written guidance. This report was generated according to the requirements of *Technical Work Plan for: Near-Field Environment and Transport In-Drift Geochemistry Model Report Integration* (BSC 2004 [DIRS 171156]), as directed by AP-2.27Q.

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- 10 CFR 63. Energy: Disposal of High-Level Radioactive Wastes in a Geologic Repository at Yucca Mountain, Nevada. Readily available. 156605
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9.3 SOURCE DATA, LISTED BY DATA TRACKING NUMBER

- GS020408312272.003. Collection and Analysis of Pore Water Samples for the Period from April 2001 to February 2002. Submittal date: 04/24/2002. 160899
- GS020808312272.004. Analysis of Water-Quality Samples for the Period from July 1999 to July 2002. Submittal date: 09/18/2002. 166569
- GS030408312272.002. Analysis of Water-Quality Samples for the Period from July 2002 to November 2002. Submittal date: 05/07/2003. 165226
- GS031008312272.008. Analysis of Pore Water and Miscellaneous Water Samples for the Period from December 2002 to July 2003. Submittal date: 11/13/2003. 166570

LB0302DSCPTHCS.002. Drift-Scale Coupled Processes (THC Seepage) Model: Data Summary. Submittal date: 02/11/2003.	161976
LL000320405924.146. Target Compositions of Aqueous Solutions Used for Corrosion Testing. Submittal date: 03/22/2000.	148327
LL031106231032.007. High Temperature Solubility and Vapor Pressure (Relative Humidity) Data for Aqueous Systems Containing Single and Multiple Salts. Submittal date: 11/19/2003.	170605
LL980704605924.035. Engineering Material Characterization Report, Volume 3. Submittal date: 07/17/1998.	147298
MO0005PORWATER.000. Perm-Sample Pore Water Data. Submittal date: 05/04/2000.	150930
MO0207EBSDUSTS.020. Geochemical Composition of Dust Samples. Submittal date: 07/11/2002.	162556
MO0209EBSDUST2.030. Geochemical Composition of Dust Samples (Phase II). Submittal date: 09/30/2002.	162557
MO0210MWDEXC01.008. CSNF Results in Excel Spreadsheets - CSNF_Spreadsheets. Submittal date: 10/22/2002.	163531
MO0302SPATHDYN.000. Thermodynamic Data Input Files - Data0.YMP.R2. Submittal date: 02/05/2003.	161756
MO0303MWDIOJ13.000. Example EQ3/6 In-Drift Precipitates/Salts Model Input/Output Files for In Situ J-13 Well Water. Submittal date: 03/04/2003.	162841
MO0303SPAMEQ36.000. General Formats of In-Drift Precipitates/Salts Model EQ3/6 Input Files. Submittal date: 03/04/2003.	162549
MO0312SPAESMUN.002. Estimated Model Uncertainties in IDPS Model Outputs. Submittal date: 12/03/2003.	166329
MO0312SPAPCEML.003. EBS P&CE Model Longevity of Materials Evaluation. Submittal date: 12/18/2003.	167409
MO0406SEPTVDST.000. Temperature and Volume Water Content for Drift Scale Test (DST) Heating Phase for Boreholes 79 and 80. Submittal date: 06/29/2004.	170616
MO0407SEPFEPLA.000. LA FEP List. Submittal date: 07/20/2004.	170760
MO0409MWDUGCMW.000. Updated General Corrosion Model of the Waste Package Outer Barrier. Submittal date: 09/17/2004.	171714

MO0409SPAACRWP.000. Aqueous Corrosion Rates For Non-Waste Form Waste Package Materials. Submittal date: 09/16/2004. 172059

SN0302T0510102.002. Pitzer Thermodynamic Database (data0.ypf, Revision 1). Submittal date: 02/06/2003. 162572

9.4 OUTPUT DATA, LISTED BY DATA TRACKING NUMBER

MO0303MWDEBSSM.000. EBS Abstraction of the THC Seepage Model: Binning Analysis Evaporation to 65% RH EQ6 Input and Output Files. Submittal date: 03/12/2003.

MO0303MWDSCMAB.000. THC Seepage Chemistry Model Abstraction Binning EQ3 Input, Pickup and Output Files. Submittal date: 03/06/2003.

MO0304MWDEBSSA.000. EBS THC Seepage Abstraction TSPA-LA Lookup Table EQ6 Input and Output Files. Submittal date: 04/01/2003.

MO0304MWDSAB11.001. EBS THC Seepage Abstraction 11 Bin EQ3 3i, 3p, and 3o Files. Submittal date: 04/08/2003.

MO0304SPAA11GC.000. EBS THC Seepage Abstraction 11 Bin EQ3 3o File Water and Gas Chemistry Extraction. Submittal date: 04/10/2003.

MO0304SPACPSLT.000. Combined In-Drift Precipitates/Salts Model Lookup Table for Seepage Evaporation Abstractions for All Bins. Submittal date: 04/18/2003.

MO0304SPACSALT.000. EBS Chemistry THC Seepage Model Abstraction Lookup Tables for TSPA-LA. Submittal date: 04/14/2003.

MO0308SPACO2GL.001. EBS Environment In-Drift CO2 Gas Lookup Tables for TSPA-LA. Submittal date: 08/04/2003.

MO0310SPADLALT.001. Dust Leachate Low Temperature Lookup Tables For TSPA-LA. Submittal date: 10/15/2003.

MO0310SPADLBU4.001. Dust Leachate Binning And Uncertainty Analysis Spreadsheets. Submittal date: 10/08/2003.

MO0310SPADLHTL.000. Dust Leachate High Temperature Lookup Tables For TSPA-LA. Submittal date: 10/15/2003.

MO0310SPAEBSCB.003. EBS Chemistry Binning Abstraction Results of the THC Seepage Model. Submittal date: 10/15/2003.

MO0310SPAEBSSB.002. EBS P&CE Model THC Seepage Within and Without Bin Uncertainty Analyses. Submittal date: 10/15/2003.

MO0310SPAEBSE.002. EBS Chemistry Unevaporated Binning Abstraction Statistics. Submittal date: 10/15/2003.

MO0310SPAPCEAC.002. EBS P&CE Alternate Conceptual Model Calculations. Submittal date: 10/15/2003.

MO0310SPAPCEGS.000. EBS P&CE "Goldsim Friendly" THC Seepage Look-Up Tables For TSPA-LA. Submittal date: 10/16/2003.

MO0310SPAPCELA.002. EBS P&CE Model Dust Leachate Analyses Spreadsheets and Data. Submittal date: 10/16/2003.

MO0310SPAPCELT.000. EBS P&CE Log Transform of Uncertainty Data. Submittal date: 10/28/2003.

MO0310SPAPCEUA.002. EBS P&CE Uncertainty Analyses for pCO₂, Br, and Mineral Suppressions. Submittal date: 10/15/2003.

MO0311SPAPEMUT.000. EBS P&CE Model Uncertainty Tables For TSPA-LA. Submittal date: 11/05/2003.

MO0311SPASADLS.000. EBS P&CE Sensitivity Analyses On Dust Leachate Silica Values. Submittal date: 11/05/2003.

MO0312SPAPCESA.002. EBS P&CE Model THC Seepage Analysis Spreadsheets. Submittal date: 12/10/2003.

MO0406MWDARHPW.000. Abstraction of Repository Horizon Pore Waters using EQ3/6. Submittal date: 06/18/2004.

MO0407SPAPCEML.005. EBS P&CE Model Longevity of Materials Evaluation. Submittal date: 06/22/2004.

SN0303T0510102.004. EQ3/6 (Version 8.0) Input/Output Data Files - Salt Deliquescence Point Modeling as A Function of Temperature. Submittal date: 04/29/2003.

SN0310T0510102.010. Analysis Of In-Drift Dust Leachates At 25 Degrees C To Various Evaporation Relative Humidity (RH) Levels. Submittal date: 10/08/2003.

SN0310T0510102.011. Dust Leachate Abstraction TSPA-LA Lookup Table EQ3/6 Input And Output Files, Low Temperature. Submittal date: 10/14/2003.

SN0310T0510102.012. Dust Leachate Abstraction TSPA-LA Lookup Table EQ3/6 Input And Output Files, High Temperature. Submittal date: 10/14/2003.

SN0312T0510102.013. EBS P&CE Model Stainless Steel Abstraction. Submittal date: 12/15/2003.

SN0403T0503404.001. Maximum Relative Humidity (RH) of Halite Precipitation Extracted from P&CE Seepage Evaporation Look-Up Tables. Submittal date: 03/24/2004.

SN0404T0510102.014. Sierra Nevada Spring Water Validation; EQ3/6 Runs and Results. Submittal date: 04/19/2004.

SN0406T0510102.015. EBS P&CE Model Validation of Interpolation Calculations. Submittal date: 06/14/2004.

SN0407T0510102.017. EBS P&CE Model Gas Flux Evaluation. Submittal date: 07/16/2004.

9.5 SOFTWARE CODES

BSC (Bechtel SAIC Company) 2003. <i>Software Code: EQ3/6</i> . V8.0. PC w/ Windows 95/98/2000/NT 4.0. 10813-8.0-00.	162228

BSC 2003. <i>Software Code: GetEQData</i> . V1.0.1. PC w/Windows 2000. 10809-1.0.1-0.	161900

BSC 2003. <i>Software Code: GoldSim</i> . V7.50.100. PC. 10344-7.50.100-00.	161572

APPENDIX A
SUPPORTING FILES ON CD ROM

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A. SUPPORTING FILES ON CD ROM

Table A-1 documents the output DTNs created by this document and lists the data files and the locations citing these DTNs. All files are date-stamped: 11/22/2004 at 9:05 AM. These .zip files are found in the attached CD ROM.

Table A-1. Traceability of Output DTNs to the Section or Table from Which They Were Developed and Their Associated Files Archived on CD ROM

Output DTN	Associated File Traceability Table or Section	File Name(s)	File Size (KB)
SN0310T0510102.010	Tables 6.10-2 and 6.10-3 Table 6.10-11 Table 6.12-5 Table 6.12-9 Sections 6.10.2 to 6.10.4 Sections 6.10.5.1 and 6.10.5.2 Section 6.10.5.5 Section 6.10.6.1 Section 6.10.8 Section 7.2.4 Table 8.2-2	<i>Dust-25c.zip</i>	12,628
MO0303MWDEBSSM.000	Table 6.6-1 Tables 6.6-13 and 6.6-14 Sections 6.6.3 and 6.6.4 Section 6.7.3 Table 8.2-2	<i>W0_THCabstractionRH65_6i_6o_files.zip</i> <i>W4_THCabstractionRH65_6i_6o_files.zip</i> <i>W5_THCabstractionRH65_6i_6o_files.zip</i> <i>W6_THCabstractionRH65_6i_6o_files.zip</i> <i>W7_THCabstractionRH65_6i_6o_files.zip</i> <i>Readme.doc</i>	8,783 8,999 9,214 8,994 9,076 19
MO0310SPADLBU4.001	Table 6.7-7 Tables 6.10-4 to 6.10-10 Table 6.12-5 Section 6.7.4 Section 6.10.4 Sections 6.10.5.2 and 6.10.5.3 Section 6.10.5.5 Section 7.2.4 Table 8.2-1	<i>DustLeachateBinning_Uncertainty.zip</i>	232
MO0303MWDSCMAB.000	Table 6.6-1 Section 6.6.3 Section 6.7.3 Section 6.9.1 Table 8.2-2	<i>W0_THCabstraction3i3o3pfiles.zip</i> <i>W4_THCabstraction3i3o3pfiles.zip</i> <i>W5_THCabstraction3i3o3pfiles.zip</i> <i>W6_THCabstraction3i3o3pfiles.zip</i> <i>W7_THCabstraction3i3o3pfiles.zip</i> <i>Readme.doc</i>	1,232 1,260 2,488 2,464 2,522 19
MO0310SPAEB SUE.002	Section 6.12.3.1 Section 7.2.1 Table 8.2-2	<i>New_Non_Evaporated_Binning_Statistics02.zip</i>	283

Table A-1. Traceability of Output DTNs to the Section or Table from Which They Were Developed and Their Associated Files Archived on CD ROM (Continued)

Output DTN	Associated File Traceability Table or Section	File Name(s)	File Size (KB)
SN0310T0510102.011	Tables 6.10-12 and 6.10-13 Table 6.12-9 Section 6.10.6 Sections 6.10.6.2 and 6.10.6.3 Table 8.2-2	<i>Dust_040C.zip</i> <i>Dust_070.zip</i> <i>Dust_100C.zip</i> <i>readme.txt</i>	1,664 1,745 2,305 1
SN0310T0510102.012	Tables 6.10-12 and 6.10-13 Section 6.10.6 Sections 6.10.6.2 and 6.10.6.3 Table 8.2-2	<i>Dust_120C.zip</i> <i>Dust_140C.zip</i> <i>Dust_150C.zip</i> <i>ReadMe.txt</i>	2,204 1,955 1,189 1
MO0304MWDEBSSA.000	Table 6.9-5 Table 6.12-9 Section 6.9.2 Section 7.2.2 Table 8.2-2	<i>EQ6_Cond.zip</i> <i>EQ6_EVAP.zip</i> <i>Readme.doc</i>	5,387 17,658 20
MO0304MWDSAB11.001	Tables 6.9-3 and 6.9-4 Table 6.12-9 Section 6.8.2 Section 6.8.4.1 Section 6.9.1 Section 6.12.4.1.3 Table 8.2-2	<i>11_Bin3i3p3o_files.zip</i> <i>Readme.doc</i>	183 20
MO0304SPAA11GC.000	Tables 6.7-6 Tables 6.9-1 and 6.9-2 Section 6.9.1 Table 8.2-2	<i>11_bin_EQ3_file_dataExtract.zip</i>	12
MO0308SPACO2GL.001	Tables 6.7-1 to 6.7-5 Sections 6.7.2.1 and 6.7.2.2 Section 6.12.5.3 Section 6.13.2.1 Section 6.15.1.1 Section 6.15.2 Table 8.2-1	<i>CO2LookupTables.zip</i>	48
MO0304SPACPSLT.000	Section 6.13.1.2 Table 8.2-2	<i>checked_MOALT_r1.zip</i>	6,799

Table A-1. Traceability of Output DTNs to the Section or Table from Which They Were Developed and Their Associated Files Archived on CD ROM (Continued)

Output DTN	Associated File Traceability Table or Section	File Name(s)	File Size (KB)
MO0304SPACSALT.000	Table 6.9-6	<i>Cond_Look-up-Tables.zip</i>	1,900
	Table 6.9-7	<i>Evap_Look-up-Tables.zip</i>	10,179
	Section 6.9.3	<i>Readme.doc</i>	20
	Section 6.12.5		
	Section 6.12.5.3		
	Section 6.15.1.1		
	Section 6.15.2		
MO0310SPADLALT.001	Table 8.2-1		
	Section 8.2.1		
	Table 6.10-14	<i>Low_Temp_Dust_Lookup_Tables.zip</i>	4,956
	Section 6.10.6.5		
	Section 6.10.8		
	Section 6.12.5		
MO0310SPAEBSCB.003	Section 6.12.5.2 and 6.12.5.3		
	Section 6.15.1.2		
	Table 8.2-1		
	Tables 6.6-3 to 6.6-14	<i>Incomplete_65%_RH_EQ6_files.zip</i>	624
	Sections 6.6.4 to 6.6.6	<i>pCO2and65percentRHBinAbstractionReruns.zip</i>	1,763
	Sections 6.6.7.1 and 6.6.7.2	<i>Final_Checked_EBS_THC_Seepage_Binning_Abstraction_REV_4.zip</i>	585
	Section 6.11.1.1		
	Section 6.12.3.1		
	Section 6.15.1.1		
	Section 6.15.2		
MO0310SPAPCEAC.002	Section 7.2.1		
	Table 8.2-1		
	Tables 6.11-1 to 6.11-14	<i>Alternative_Conceptual_Model_Statistics.zip</i>	533
MO0310SPAPCELA.002	Section 6.11.1.1		
	Table 8.2-2		
	Tables 6.13-7 and 6.13-9	<i>Dust_Leach_anal_spreadsheets.zip</i>	7,275
	Section 6.12.4.2.4		
	Sections 6.13.2.1 to 6.13.2.3		
	Section 6.13.4.2		
	Table 8.2-2		

Table A-1. Traceability of Output DTNs to the Section or Table from Which They Were Developed and Their Associated Files Archived on CD ROM (Continued)

Output DTN	Associated File Traceability Table or Section	File Name(s)	File Size (KB)
MO0407SPAPCEML.005	Table 4.1-2 Tables 6.4-11, 6.4-15, and 6.4-18 Section 4.1.1 Table 8.2-2	<i>Longevity.zip</i>	11
MO0312SPAPCESA.002	Tables 6.13-1, 6.13-2, 6.13-6, and 6.13-8 Section 6.13 Sections 6.13.1.3, 6.13.4.1, and 6.13.5.2 Section 7.2.1 Table 8.2-2	<i>THCSeepageModelAnalysis.zip</i>	8,110
MO0310SPAEBSSB.002	Section 6.12.3.1 Table 8.2-2	<i>RH98andRH85EQ6filesW0.zip</i> <i>RH98andRH85EQ6filesW4.zip</i> <i>RH98andRH85EQ6filesW5.zip</i> <i>RH98andRH85EQ6filesW6.zip</i> <i>RH98andRH85EQ6filesW7.zip</i> <i>THC_Seepage_Bin_Uncertainty.zip</i>	10,464 11,193 11,165 11,202 10,879 771
SN0312T0510102.013	Tables 4.1-23 and 4.1-24 Tables 6.8-2 and 6.8-5 Tables 6.12-10 to 6.12-19 Sections 6.8.2 and 6.8.3 Sections 6.8.4.1 and 6.8.4.3 Section 6.12.4.1 Table 8.2-2	<i>Base case.zip</i> <i>DegradationMolality.zip</i> <i>Cr-database.zip</i> <i>Cr-validation.zip</i> <i>Uncertainties.zip</i> <i>readme.txt</i>	376 9 2 81 1758 2
MO0310SPAPCEUA.002	Tables 6.12-21 to 6.12-28 Section 6.12.4.2.4 Sections 6.12.4.3.2 and 6.12.4.3.3 Section 6.12.4.4 Sections 6.12.4.1.1 and 6.12.4.4.2 Table 8.2-2	<i>DustLeachBrSensitivity.zip</i> <i>MineralSuppressions.zip</i> <i>PCO2DustLeachSensitivity.zip</i> <i>seepage_pco2uncertcalcs.zip</i> <i>SeepageBrSensitivityStudy.zip</i>	289 675 666 972 4,075
SN0404T0510102.014	Section 7.3 Table 8.2-2	<i>sierra.zip</i>	97
SN0303T0510102.004	Tables 7.4-1 and 7.4-2 Table 8.2-2	<i>Salt_Deliq_EQ36_IO_files.zip</i>	363

Table A-1. Traceability of Output DTNs to the Section or Table from Which They Were Developed and Their Associated Files Archived on CD ROM (Continued)

Output DTN	Associated File Traceability Table or Section	File Name(s)	File Size (KB)
MO0310SPADLHTL.000	Table 6.10-14 Section 6.10.6.5 Section 6.12.5 Section 6.12.5.2 and 6.12.5.3 Section 6.15.1.2 Table 8.2-1	<i>High_T_Dust_Lookup_Tables.zip</i>	3,459
MO0310SPAPCEGS.000	Tables 6.9-6 and 6.9-7 Sections 6.9.3 and 6.9.4 Section 6.11.2 Section 6.12.5 Sections 6.12.5.2 and 6.12.5.3 Section 6.15.1.1 Section 6.15.2 Section 7.2.1 Section 8.2.1 Section 8.2.1	<i>seepage_lookup_cond.zip</i> <i>seepage_lookup_evap.zip</i> <i>Readme_cond.doc</i> <i>Readme_evap.doc</i>	1,927 10,238 20 20
MO0310SPAPCELT.000	Tables 6.12-2 and 6.12-6 Section 6.12.3.1 Table 8.2-2	<i>LogTransform.zip</i>	1,494
MO0311SPAEPMT.000	Tables 6.12-4 and 6.12-8, Tables 6.12-29 and 6.12-30 Table 8.2-1	<i>TSPA_LA_UncertaintyTables.zip</i>	461
MO0311SPASADLS.000	Section 6.10.8 Table 8.2-2	<i>EQ36_SiO2_sensitivity_analysis.zip</i>	777
MO0406MWDARHPW.000	Section 7.2.3 Table 7.2-1 Table 8.2-2	<i>RepositoryHorizonPoreWaters.zip</i>	2,999
SN0403T0503404.001	Section 4.1.5 Section 6.11.2 Table 8.2-1	<i>Halite_RH.zip</i>	10
SN0406T0510102.015	Section 7.2.2 Table 8.2-2	<i>InterpolationValidation.zip</i>	166
SN0407T0510102.017	Table 4.1-17 Sections 4.1.2 and 4.1.3 Sections 6.7.1.1 to 6.7.1.3 Table 8.2-2	<i>Oxygen_Evaluation.zip</i>	103

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APPENDIX B
THC SEEPAGE LOOKUP TABLE RESULTS

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B. THC SEEPAGE LOOKUP TABLE RESULTS

The graphs presented in this document are representative of the information available in DTN: MO0304SPACSALT.000. Two graphs from each excel file are shown here; they are: Aqueous Composition Evaporation Predictions vs. Relative Humidity and Mineral Precipitation Evaporation Predictions vs. Relative Humidity. Also available in this DTN: MO0304SPACSALT.000 is the condensation information: Aqueous Composition Condensation Predictions vs. Relative Humidity, Aqueous Composition Condensation Predictions vs. Concentration Factor, ANC Species Concentration Condensation Predictions vs. Relative Humidity, and ANC Species Concentration Condensation Predictions vs. Concentration Factor. This information is provided for each respective bin and parameter setting. Also available in the respective excel files, but not shown here, are: ANC Species Concentration Evaporation Predictions vs. Relative Humidity, ANC Species Concentration Evaporation Predictions vs. Concentration Factor, Aqueous Composition Evaporation Predictions vs. Concentration Factor, and Mineral Precipitation Evaporation Predictions vs. Concentration.

The graphs given in this document are referenced only by the bin number and parameter settings. Table B-1 gives the associated excel source file name for the graphs in this document. Each excel file header contains the traceability back to the specific input data used in the calculation. The file nomenclature is *d?c#t%.xls*, where d represents the dust bin, ? is the 1-digit bin number (01, 02, etc.), # = 2, 3, or 4 (for $p\text{CO}_2 = 10^{-\#}$), % = 4, 7, or 1 (for temp = 40°C, 70°C, or 100°C, respectively). FILE NAME EXAMPLE (*d1c2t1.xls*) dust bin 01 at a $p\text{CO}_2$ of 10^{-2} at 100°C.

For the figures shown below, two terms need to be defined:

1. IS: Ionic Strength
2. RH: Relative Humidity.

The values in Table B-2 correspond to the given parameters extracted from the excel files in DTN: MO0304SPACSALT.000. Given in this table are deliquescence point relative humidity and the associated chemical parameters of interest to TSPA.

Table B-1. Excel File Names for Each Lookup Table in DTN: MO0304SPACSALT.000

Bin	Evaporation Lookup Tables	Condensation Lookup Tables
1	01c2t1e.xls.xls, 01c3t1e.xls.xls, 01c4t1e.xls.xls, 01c2t4e.xls.xls, 01c3t4e.xls.xls, 01c4t4e.xls.xls, 01c2t7e.xls.xls, 01c3t7e.xls.xls, 01c4t7e.xls.xls	01c2t1c.xls.xls, 01c3t1c.xls.xls, 01c4t1c.xls.xls, 01c2t4c.xls.xls, 01c3t4c.xls.xls, 01c4t4c.xls.xls, 01c2t7c.xls.xls, 01c3t7c.xls.xls, 01c4t7c.xls.xls
2	02c2t1e.xls.xls, 02c3t1e.xls.xls, 02c4t1e.xls.xls, 02c2t4e.xls.xls, 02c3t4e.xls.xls, 02c4t4e.xls.xls, 02c2t7e.xls.xls, 02c3t7e.xls.xls, 02c4t7e.xls.xls	02c2t1c.xls.xls, 02c3t1c.xls.xls, 02c4t1c.xls.xls, 02c2t4c.xls.xls, 02c3t4c.xls.xls, 02c4t4c.xls.xls, 02c2t7c.xls.xls, 02c3t7c.xls.xls, 02c4t7c.xls.xls
3	03c2t1e.xls.xls, 03c3t1e.xls.xls, 03c4t1e.xls.xls, 03c2t4e.xls.xls, 03c3t4e.xls.xls, 03c4t4e.xls.xls, 03c2t7e.xls.xls, 03c3t7e.xls.xls, 03c4t7e.xls.xls	03c2t1c.xls.xls, 03c3t1c.xls.xls, 03c4t1c.xls.xls, 03c2t4c.xls.xls, 03c3t4c.xls.xls, 03c4t4c.xls.xls, 03c2t7c.xls.xls, 03c3t7c.xls.xls, 03c4t7c.xls.xls
4	04c2t1e.xls.xls, 04c3t1e.xls.xls, 04c4t1e.xls.xls, 04c2t4e.xls.xls, 04c3t4e.xls.xls, 04c4t4e.xls.xls, 04c2t7e.xls.xls, 04c3t7e.xls.xls, 04c4t7e.xls.xls	04c2t1c.xls.xls, 04c3t1c.xls.xls, 04c4t1c.xls.xls, 04c2t4c.xls.xls, 04c3t4c.xls.xls, 04c4t4c.xls.xls, 04c2t7c.xls.xls, 04c3t7c.xls.xls, 04c4t7c.xls.xls
5	05c2t1e.xls.xls, 05c3t1e.xls.xls, 05c4t1e.xls.xls, 05c2t4e.xls.xls, 05c3t4e.xls.xls, 05c4t4e.xls.xls, 05c2t7e.xls.xls, 05c3t7e.xls.xls, 05c4t7e.xls.xls	05c2t1c.xls.xls, 05c3t1c.xls.xls, 05c4t1c.xls.xls, 05c2t4c.xls.xls, 05c3t4c.xls.xls, 05c4t4c.xls.xls, 05c2t7c.xls.xls, 05c3t7c.xls.xls, 05c4t7c.xls.xls
6	06c2t1e.xls.xls, 06c3t1e.xls.xls, 06c4t1e.xls.xls, 06c2t4e.xls.xls, 06c3t4e.xls.xls, 06c4t4e.xls.xls, 06c2t7e.xls.xls, 06c3t7e.xls.xls, 06c4t7e.xls.xls	06c2t1c.xls.xls, 06c3t1c.xls.xls, 06c4t1c.xls.xls, 06c2t4c.xls.xls, 06c3t4c.xls.xls, 06c4t4c.xls.xls, 06c2t7c.xls.xls, 06c3t7c.xls.xls, 06c4t7c.xls.xls
7	07c2t1e.xls.xls, 07c3t1e.xls.xls, 07c4t1e.xls.xls, 07c2t4e.xls.xls, 07c3t4e.xls.xls, 07c4t4e.xls.xls, 07c2t7e.xls.xls, 07c3t7e.xls.xls, 07c4t7e.xls.xls	07c2t1c.xls.xls, 07c3t1c.xls.xls, 07c4t1c.xls.xls, 07c2t4c.xls.xls, 07c3t4c.xls.xls, 07c4t4c.xls.xls, 07c2t7c.xls.xls, 07c3t7c.xls.xls, 07c4t7c.xls.xls
8	08c2t1e.xls.xls, 08c3t1e.xls.xls, 08c4t1e.xls.xls, 08c2t4e.xls.xls, 08c3t4e.xls.xls, 08c4t4e.xls.xls, 08c2t7e.xls.xls, 08c3t7e.xls.xls, 08c4t7e.xls.xls	08c2t1c.xls.xls, 08c3t1c.xls.xls, 08c4t1c.xls.xls, 08c2t4c.xls.xls, 08c3t4c.xls.xls, 08c4t4c.xls.xls, 08c2t7c.xls.xls, 08c3t7c.xls.xls, 08c4t7c.xls.xls
9	09c2t1e.xls.xls, 09c3t1e.xls.xls, 09c4t1e.xls.xls, 09c2t4e.xls.xls, 09c3t4e.xls.xls, 09c4t4e.xls.xls, 09c2t7e.xls.xls, 09c3t7e.xls.xls, 09c4t7e.xls.xls	09c2t1c.xls.xls, 09c3t1c.xls.xls, 09c4t1c.xls.xls, 09c2t4c.xls.xls, 09c3t4c.xls.xls, 09c4t4c.xls.xls, 09c2t7c.xls.xls, 09c3t7c.xls.xls, 09c4t7c.xls.xls
10	10c2t1e.xls.xls, 10c3t1e.xls.xls, 10c4t1e.xls.xls, 10c2t4e.xls.xls, 10c3t4e.xls.xls, 10c4t4e.xls.xls, 10c2t7e.xls.xls, 10c3t7e.xls.xls, 10c4t7e.xls.xls	10c2t1c.xls.xls, 10c3t1c.xls.xls, 10c4t1c.xls.xls, 10c2t4c.xls.xls, 10c3t4c.xls.xls, 10c4t4c.xls.xls, 10c2t7c.xls.xls, 10c3t7c.xls.xls, 10c4t7c.xls.xls
11	11c2t1e.xls.xls, 11c3t1e.xls.xls, 11c4t1e.xls.xls, 11c2t4e.xls.xls, 11c3t4e.xls.xls, 11c4t4e.xls.xls, 11c2t7e.xls.xls, 11c3t7e.xls.xls, 11c4t7e.xls.xls	11c2t1c.xls.xls, 11c3t1c.xls.xls, 11c4t1c.xls.xls, 11c2t4c.xls.xls, 11c3t4c.xls.xls, 11c4t4c.xls.xls, 11c2t7c.xls.xls, 11c3t7c.xls.xls, 11c4t7c.xls.xls

Source: DTN: MO0304SPACSALT.000.

Table B-2. Deliquescence Point Relative Humidity and Associated Chemical Parameters Taken from the THC Seepage Lookup Tables in DTN: MO0304SPACSALT.000

Bin	Temperature (°C)	pCO ₂ (bars)	Deliquescence Point Relative Humidity	pH	Ionic Strength (Moles/kg. H ₂ O)	Cl (Moles/kg. H ₂ O)	NO ₃ (Moles/kg. H ₂ O)
1	100	0.0100	20.037%	3.817	3.985E+01	2.513E+01	1.989E-00
	40		18.119%	3.572	3.736E+01	2.406E+01	1.313E-00
	70		18.692%	3.646	3.864E+01	2.431E+01	1.938E-00
	100	0.0010	20.038%	4.317	3.985E+01	2.512E+01	1.990E-00
	40		18.062%	4.018	3.556E+01	2.266E+01	1.485E-00
	70		18.704%	4.146	3.866E+01	2.432E+01	1.937E-00
	100	0.0001	20.013%	4.816	3.984E+01	2.511E+01	1.989E-00
	40		18.245%	4.493	3.441E+01	2.174E+01	1.607E-00
	70		18.685%	4.645	3.864E+01	2.430E+01	1.937E-00
2	100	0.0100	24.000%	4.423	3.624E+01	2.126E+01	4.690E-00
	40		23.135%	4.597	3.763E+01	2.192E+01	4.904E-00
	70		23.412%	4.381	3.540E+01	2.066E+01	4.619E-00
	100	0.0010	24.000%	4.921	3.620E+01	2.123E+01	4.684E-00
	40		23.137%	5.096	3.762E+01	2.191E+01	4.905E-00
	70		24.000%	4.806	3.358E+01	1.959E+01	4.383E-00
	100	0.0001	24.000%	5.420	3.618E+01	2.122E+01	4.682E-00
	40		23.141%	5.596	3.763E+01	2.191E+01	4.902E-00
	70		24.000%	5.306	3.358E+01	1.958E+01	4.382E-00
3	100	0.0100	43.947%	4.906	2.038E+01	1.317E+01	3.620E-00
	40		38.942%	4.441	2.000E+01	1.221E+01	2.382E-00
	70		42.259%	4.736	2.024E+01	1.166E+01	4.312E-00
	100	0.0010	44.004%	5.415	2.039E+01	1.323E+01	3.597E-00
	40		39.781%	4.972	1.975E+01	1.208E+01	2.373E-00
	70		42.471%	5.265	2.024E+01	1.180E+01	4.237E-00
	100	0.0001	44.020%	5.915	2.039E+01	1.323E+01	3.595E-00
	40		39.953%	5.488	1.973E+01	1.209E+01	2.373E-00
	70		42.492%	5.767	2.024E+01	1.181E+01	4.230E-00
4	100	0.0100	47.411%	6.473	2.239E+01	3.936E-00	1.523E+01
	40		65.012%	6.325	1.346E+01	3.994E-00	8.100E-00
	70		52.860%	6.049	2.029E+01	1.904E-00	1.705E+01
	100	0.0010	47.412%	6.973	2.239E+01	3.937E-00	1.523E+01
	40		65.014%	6.825	1.346E+01	3.994E-00	8.101E-00
	70		52.861%	6.549	2.029E+01	1.902E-00	1.705E+01
	100	0.0001	47.414%	7.473	2.239E+01	3.936E-00	1.523E+01
	40		65.014%	7.325	1.346E+01	3.994E-00	8.101E-00
	70		52.861%	7.048	2.029E+01	1.900E-00	1.705E+01
5	100	0.0100	60.130%	7.270	1.727E+01	8.186E-00	1.802E-00
	40		69.130%	7.119	1.001E+01	5.998E-00	1.321E-00
	70		62.053%	7.136	1.660E+01	6.375E-00	3.728E-00
	100	0.0010	60.129%	7.770	1.728E+01	8.186E-00	1.801E-00
	40		69.943%	7.637	9.368E-00	6.267E-00	7.024E-01
	70		62.066%	7.636	1.658E+01	6.375E-00	3.726E-00
	100	0.0001	60.131%	8.269	1.727E+01	8.182E-00	1.801E-00
	40		62.351%	7.880	1.996E+01	3.406E-00	8.532E-00
	70		62.059%	8.136	1.659E+01	6.376E-00	3.726E-00

Table B-2. Deliquescence Point Relative Humidity and Associated Chemical Parameters Taken from the THC Seepage Lookup Tables in DTN: MO0304SPACSALT.000 (Continued)

Bin	Temperature (°C)	pCO ₂ (bars)	Deliquescence Point Relative Humidity	pH	Ionic Strength (Moles/kg. H ₂ O)	Cl (Moles/kg. H ₂ O)	NO ₃ (Moles/kg. H ₂ O)
6	100	0.0100	59.117%	8.999	1.719E+01	7.213E-00	2.518E-00
	40		62.976%	8.298	1.979E+01	4.304E-00	6.088E-00
	70		60.500%	8.910	1.782E+01	5.750E-00	4.430E-00
	100	0.0010	59.123%	9.503	1.717E+01	7.269E-00	2.440E-00
	40		61.745%	9.266	2.055E+01	3.930E-00	6.918E-00
	70		59.703%	9.510	1.854E+01	5.458E-00	5.018E-00
	100	0.0001	58.888%	9.999	1.730E+01	7.200E-00	2.207E-00
	40		64.071%	10.096	1.404E+01	5.033E-00	2.567E-00
	70		59.630%	10.010	1.856E+01	5.458E-00	4.897E-00
7	100	0.0100	59.108%	8.999	1.720E+01	7.215E-00	2.519E-00
	40		62.976%	8.298	1.979E+01	4.304E-00	6.088E-00
	70		60.501%	8.910	1.781E+01	5.750E-00	4.430E-00
	100	0.0010	59.123%	9.503	1.717E+01	7.269E-00	2.440E-00
	40		61.745%	9.266	2.054E+01	3.930E-00	6.918E-00
	70		59.704%	9.510	1.854E+01	5.458E-00	5.018E-00
	100	0.0001	60.000%	9.992	1.607E+01	7.120E-00	1.835E-00
	40		66.234%	10.126	1.237E+01	5.606E-00	7.012E-01
	70		59.634%	10.010	1.855E+01	5.457E-00	4.896E-00
8	100	0.0100	59.112%	8.999	1.720E+01	7.214E-00	2.518E-00
	40		62.977%	8.298	1.978E+01	4.304E-00	6.088E-00
	70		60.498%	8.910	1.782E+01	5.751E-00	4.430E-00
	100	0.0010	59.116%	9.503	1.718E+01	7.270E-00	2.441E-00
	40		61.744%	9.266	2.055E+01	3.930E-00	6.918E-00
	70		59.701%	9.510	1.854E+01	5.458E-00	5.019E-00
	100	0.0001	58.884%	9.999	1.730E+01	7.200E-00	2.208E-00
	40		62.162%	10.061	1.594E+01	4.489E-00	4.609E-00
	70		59.624%	10.010	1.857E+01	5.459E-00	4.898E-00
9	100	0.0100	50.935%	9.157	3.012E+01	9.899E-00	8.991E-00
	40		62.013%	8.327	1.923E+01	4.532E-00	6.774E-00
	70		50.023%	9.191	3.284E+01	9.339E-00	1.075E+01
	100	0.0010	50.905%	9.661	3.017E+01	9.977E-00	8.948E-00
	40		61.329%	9.270	2.041E+01	3.934E-00	7.178E-00
	70		57.507%	9.530	2.168E+01	5.656E-00	6.710E-00
	100	0.0001	52.305%	10.061	2.794E+01	8.008E-00	8.526E-00
	40		62.119%	10.060	1.593E+01	4.479E-00	4.590E-00
	70		49.783%	10.274	3.307E+01	9.401E-00	1.070E+01
10	100	0.0100	58.991%	8.997	1.724E+01	7.175E-00	2.556E-00
	40		66.105%	8.399	1.247E+01	5.578E-00	2.558E-00
	70		60.345%	8.907	1.787E+01	5.704E-00	4.485E-00
	100	0.0010	59.008%	9.501	1.721E+01	7.229E-00	2.477E-00
	40		61.525%	9.262	2.061E+01	3.879E-00	7.010E-00
	70		59.598%	9.508	1.857E+01	5.428E-00	5.056E-00
	100	0.0001	58.844%	9.996	1.725E+01	7.147E-00	2.235E-00
	40		62.119%	10.060	1.593E+01	4.480E-00	4.589E-00
	70		59.542%	10.008	1.856E+01	5.424E-00	4.932E-00

Table B-2. Deliquescence Point Relative Humidity and Associated Chemical Parameters Taken from the THC Seepage Lookup Tables in DTN: MO0304SPACSALT.000 (Continued)

Bin	Temperature (°C)	pCO ₂ (bars)	Deliquescence Point Relative Humidity	pH	Ionic Strength (Moles/kg. H ₂ O)	Cl (Moles/kg. H ₂ O)	NO ₃ (Moles/kg. H ₂ O)
11	100	0.0100	58.995%	8.997	1.723E+01	7.174E-00	2.555E-00
	40		62.683%	8.292	1.995E+01	4.227E-00	6.213E-00
	70		60.351%	8.907	1.786E+01	5.703E-00	4.484E-00
	100	0.0010	59.004%	9.501	1.721E+01	7.229E-00	2.477E-00
	40		61.524%	9.262	2.062E+01	3.879E-00	7.011E-00
	70		59.596%	9.508	1.858E+01	5.428E-00	5.056E-00
	100	0.0001	58.768%	9.997	1.734E+01	7.160E-00	2.245E-00
	40		62.119%	10.060	1.593E+01	4.476E-00	4.593E-00
	70		59.511%	10.008	1.862E+01	5.430E-00	4.936E-00

Source: DTN: MO0304SPACSALT.000.

NOTE: Deliquescence Point Relative Humidity can not be confirmed in all cases (Table 6.12-1).

Source: DTN: MO0304SPACCSALT.000\01c2\1e.xls.xls.

Figure B-01-1. Bin 01 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACCSALT.000\01c2\1e.xls.xls.

Figure B-01-2. Bin 01 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACCSALT.000\01c3\1e.xls.xls.

Figure B-01-3. Bin 01 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACCSALT.000\01c3\1e.xls.xls.

Figure B-01-4. Bin 01 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\01c4t1e.xls.xls.

Figure B-01-5. Bin 01 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\01c4t1e.xls.xls.

Figure B-01-6. Bin 01 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\01c2t7e.xls.xls.

Figure B-01-7. Bin 01 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\01c2t7e.xls.xls.

Figure B-01-8. Bin 01 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000001c307e.xls.xls

Figure B-01-9. Bin 01 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000.01c317e.xls.xls

Figure B-01-10. Bin 01 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 70°C and 10⁻³ bar CO₂ Fugacity

Source: DTN: MO0304SPACSAULT.000001c4(7e.xls.xls

Figure B-01-11. Bin 01 Aqueous Composition
Evaporation Predictions vs. Relative Humidity at
70°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAIT.000\01c4f7e.xls.xls

Figure B-01-12. Bin 01 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\01c214e.xls.xls.

Figure B-01-13. Bin 01 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\01c214e.xls.xls.

Figure B-01-14. Bin 01 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\01c314e.xls.xls.

Figure B-01-15. Bin 01 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\01c314e.xls.xls.

Figure B-01-16. Bin 01 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\01c414e.xls.xls.

Figure B-01-17. Bin 01 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\01c414e.xls.xls.

Figure B-01-18. Bin 01 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\02c211e.xls.xls.

Figure B-02-1. Bin 02 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\02c211e.xls.xls.

Figure B-02-2. Bin 02 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\02c3t1e.xls.xls

Figure B-02-3. Bin 02 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\02c3t1e.xls.xls

Figure B-02-4. Bin 02 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\02c4t1e.xls.xls

Figure B-02-5. Bin 02 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\02c4t1e.xls.xls

Figure B-02-6. Bin 02 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\02c2i7e.xls.xls.

Figure B-02-7. Bin 02 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\02c2i7e.xls.xls.

Figure B-02-8. Bin 02 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\02c3i7e.xls.xls.

Figure B-02-9. Bin 02 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\02c3i7e.xls.xls.

Figure B-02-10. Bin 02 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\02c417e.xls.xls.

Figure B-02-11. Bin 02 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-4} bar CO_2 Fugacity

DTN: MO0304SPACSALT.000\02c417e.xls.xls.

Figure B-02-12. Bin 02 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\02c214e.xls.xls.

Figure B-02-13. Bin 02 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\02c214e.xls.xls.

Figure B-02-14. Bin 02 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\02c3t4e.xls.xls.

Figure B-02-15. Bin 02 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-3} bar CO_2 Fugacity

DTN: MO0304SPACSALT.000\02c3t4e.xls.xls.

Figure B-02-16. Bin 02 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\02c4t4e.xls.xls.

Figure B-02-17. Bin 02 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\02c4t4e.xls.xls.

Figure B-02-18. Bin 02 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\03c2f1e.xls.xls

Figure B-03-1. Bin 03 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\03c2f1e.xls.xls

Figure B-03-2. Bin 03 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\03c3f1e.xls.xls

Figure B-03-3. Bin 03 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\03c3f1e.xls.xls

Figure B-03-4. Bin 03 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACCSALT.000\03c4t1e.xls.xls.

Figure B-03-5. Bin 03 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACCSALT.000\03c4t1e.xls.xls.

Figure B-03-6. Bin 03 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACCSALT.000\03c2t7e.xls.xls.

Figure B-03-7. Bin 03 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACCSALT.000\03c2t7e.xls.xls.

Figure B-03-8. Bin 03 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\03c3i7e.xls.xls

Figure B-03-9. Bin 03 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\03c3i7e.xls.xls

Figure B-03-10. Bin 03 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\03c4i7e.xls.xls

Figure B-03-11. Bin 03 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\03c4i7e.xls.xls

Figure B-03-12. Bin 03 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACCSALT.000\03c214e.xls.xls

Figure B-03-13. Bin 03 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACCSALT.000\03c214e.xls.xls

Figure B-03-14. Bin 03 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACCSALT.000\03c314e.xls.xls

Figure B-03-15. Bin 03 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACCSALT.000\03c314e.xls.xls

Figure B-03-16. Bin 03 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\03c4t4e.xls.xls

Figure B-03-17. Bin 03 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\03c4t4e.xls.xls

Figure B-03-18. Bin 03 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\04c2t1e.xls.xls

Figure B-04-1. Bin 04 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\04c2t1e.xls.xls

Figure B-04-2. Bin 04 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\04c3f1e.xls.xls.

Figure B-04-3. Bin 04 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\04c3f1e.xls.xls.

Figure B-04-4. Bin 04 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\04c4f1e.xls.xls.

Figure B-04-5. Bin 04 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\04c4f1e.xls.xls.

Figure B-04-6. Bin 04 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACCSALT.000\04c2i7e.xls.xls.

Figure B-04-7. Bin 04 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACCSALT.000\04c2i7e.xls.xls.

Figure B-04-8. Bin 04 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACCSALT.000\04c3i7e.xls.xls.

Figure B-04-9. Bin 04 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACCSALT.000\04c3i7e.xls.xls.

Figure B-04-10. Bin 04 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\04c417e.xls.xls

Figure B-04-11. Bin 04 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\04c417e.xls.xls

Figure B-04-12. Bin 04 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\04c214e.xls.xls

Figure B-04-13. Bin 04 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\04c214e.xls.xls

Figure B-04-14. Bin 04 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-2} bar CO_2 Fugacity

Figure 1 is a line graph showing the moisture content (g/g) of various polymers as a function of relative humidity (RH) at 25°C. The x-axis represents RH from 100% to 0%, and the y-axis represents Moisture Content (g/g) from 3 to 12. The polymers shown are PE, PP, PVC, PCL, PB, PS, PMMA, PET, and PEG. PE and PP show the highest moisture content, while PEG shows the lowest.

Figure 1 is a line graph showing the pH dependence of the molar ratio of mineral species in the aqueous phase. The x-axis represents pH, ranging from 3 to 12. The y-axis represents the molar ratio, ranging from 0% to 100%. The legend identifies the following species: H_2O , H_2SiO_4 , $HSiO_3^-$, SiO_3^{2-} , H_2CO_3 , HCO_3^- , CO_3^{2-} , $H_2PO_4^-$, HPO_4^{2-} , PO_4^{3-} , H_2SiO_3 , $HSiO_2$, SiO_2 , H_2SiO_2 , $HSiO$, SiO , H_2Si , HSi , Si . The graph shows that at low pH, H_2O and H_2SiO_4 are the dominant species. As pH increases, $HSiO_3^-$ and SiO_3^{2-} become dominant. H_2CO_3 and HCO_3^- are dominant in the intermediate pH range. $H_2PO_4^-$, HPO_4^{2-} , and PO_4^{3-} are dominant at higher pH. The species H_2SiO_3 , $HSiO_2$, SiO_2 , H_2SiO_2 , $HSiO$, SiO , H_2Si , HSi , and Si are present in very small amounts across the entire pH range.

The graph plots pH (y-axis, 3 to 12) against the molar ratio of Na₂CO₃ (x-axis, 0.00 to 1.00). The legend identifies the following series: Al (solid line with circles), Fe (dashed line with circles), Cu (solid line with triangles), Zn (dashed line with triangles), Pb (solid line with squares), K (dashed line with squares), Mg (solid line with diamonds), Ni (dashed line with diamonds), Co (solid line with crosses), Na (dashed line with crosses), Si (solid line with asterisks), HCO₃Na (dashed line with asterisks), and pH (solid line). The pH of the HCO₃Na solution is constant at approximately 4. The pH of the Na solution is constant at approximately 11.5. The pH of the Al solution increases from approximately 9.5 to 11.5. The pH of the Fe solution increases from approximately 9.5 to 11.0. The pH of the Cu solution increases from approximately 9.5 to 10.5. The pH of the Zn solution increases from approximately 9.5 to 10.0. The pH of the Pb solution increases from approximately 9.5 to 9.8. The pH of the K solution increases from approximately 9.5 to 9.8. The pH of the Mg solution increases from approximately 9.5 to 9.8. The pH of the Ni solution increases from approximately 9.5 to 9.8. The pH of the Co solution increases from approximately 9.5 to 9.8. The pH of the Si solution increases from approximately 9.5 to 9.8. The pH of the HCO₃Na solution is constant at approximately 4. The pH of the Na solution is constant at approximately 11.5.

Source: DTN: MO0304SPACSALT.000\05c2\1e.xls.xls

Figure B-05-1. Bin 05 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\05c2\1e.xls.xls

Figure B-05-2. Bin 05 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\05c3\1e.xls.xls

Figure B-05-3. Bin 05 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\05c3\1e.xls.xls

Figure B-05-4. Bin 05 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\05c4t1e.xls.xls.

Figure B-05-5. Bin 05 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\05c4t1e.xls.xls.

Figure B-05-6. Bin 05 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\05c2t7e.xls.xls.

Figure B-05-7. Bin 05 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\05c2t7e.xls.xls.

Figure B-05-8. Bin 05 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPAC3ALT.000\05c3i7e.xls.xls

Figure B-05-9. Bin 05 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPAC3ALT.000\05c3i7e.xls.xls

Figure B-05-10. Bin 05 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPAC3ALT.000\05c4i7e.xls.xls

Figure B-05-11. Bin 05 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPAC3ALT.000\05c4i7e.xls.xls

Figure B-05-12. Bin 05 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACCSALT.000\05c214e.xls.xls.

Figure B-05-13. Bin 05 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACCSALT.000\05c214e.xls.xls.

Figure B-05-14. Bin 05 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACCSALT.000\05c314e.xls.xls.

Figure B-05-15. Bin 05 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACCSALT.000\05c314e.xls.xls.

Figure B-05-16. Bin 05 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000V05c44e.xls.xls

Figure B-05-18. Bin 05 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 40°C and 10⁻⁴ bar CO₂ Fugacity

Source: DTN: MO0304SPACSALT.000:06c2f1e.xls.xls

Figure B-06-2. Bin 06 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\06c3\1e.xls.xls

Figure B-06-3. Bin 06 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\06c3\1e.xls.xls

Figure B-06-4. Bin 06 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\06c4\1e.xls.xls

Figure B-06-5. Bin 06 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\06c4\1e.xls.xls

Figure B-06-6. Bin 06 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\06c2\7e.xls.xls

Figure B-06-7. Bin 06 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\06c2\7e.xls.xls

Figure B-06-8. Bin 06 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\06c3\7e.xls.xls

Figure B-06-9. Bin 06 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\06c3\7e.xls.xls

Figure B-06-10. Bin 06 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\06c4f7e.xls.xls

Figure B-06-11. Bin 06 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\06c4f7e.xls.xls

Figure B-06-12. Bin 06 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\06c2f4e.xls.xls

Figure B-06-13. Bin 06 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\06c2f4e.xls.xls

Figure B-06-14. Bin 06 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\06c3t4e.xls.xls

Figure B-06-15. Bin 06 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\06c3t4e.xls.xls

Figure B-06-16. Bin 06 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\06c4t4e.xls.xls

Figure B-06-17. Bin 06 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\06c4t4e.xls.xls

Figure B-06-18. Bin 06 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-4} bar CO_2 Fugacity

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Source: DTN: MO0304SPACSAULT.000\07c411e.xls.xls

Figure B-07-5. Bin 07 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\07c411e.xls.xls

Figure B-07-6. Bin 07 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\07c217e.xls.xls

Figure B-07-7. Bin 07 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\07c217e.xls.xls

Figure B-07-8. Bin 07 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\07c3f7e.xls.xls

Figure B-07-9. Bin 07 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\07c3f7e.xls.xls

Figure B-07-10. Bin 07 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\07c4f7e.xls.xls

Figure B-07-11. Bin 07 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\07c4f7e.xls.xls

Figure B-07-12. Bin 07 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\07c2t4e.xls.xls

Figure B-07-13. Bin 07 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\07c2t4e.xls.xls

Figure B-07-14. Bin 07 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\07c3t4e.xls.xls

Figure B-07-15. Bin 07 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\07c3t4e.xls.xls

Figure B-07-16. Bin 07 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\07c4t4e.xls.xls

Figure B-07-17. Bin 07 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\07c4t4e.xls.xls

Figure B-07-18. Bin 07 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\08c2t1e.xls.xls

Figure B-08-1. Bin 08 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\08c2t1e.xls.xls

Figure B-08-2. Bin 08 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\08c3t1e.xls.xls

Figure B-08-3. Bin 08 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\08c3t1e.xls.xls

Figure B-08-4. Bin 08 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\08c4t1e.xls.xls

Figure B-08-5. Bin 08 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\08c4t1e.xls.xls

Figure B-08-6. Bin 08 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\08c2\7e.xls.xls

Figure B-08-7. Bin 08 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\08c2\7e.xls.xls

Figure B-08-8. Bin 08 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\08c3\7e.xls.xls

Figure B-08-9. Bin 08 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\08c3\7e.xls.xls

Figure B-08-10. Bin 08 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAIT.000108c4f7e.xls.xls

Figure B-08-12. Bin 08 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000108c2f4e.xls.xls

Figure B-08-14. Bin 08 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\09c2t1e.xls.xls.

Figure B-09-1. Bin 09 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\09c2t1e.xls.xls.

Figure B-09-2. Bin 09 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\09c3t1e.xls.xls.

Figure B-09-3. Bin 09 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\09c3t1e.xls.xls.

Figure B-09-4. Bin 09 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAIT.000.00c-4/1e.x/s.x/s.

Figure B-09-5. Bin 09 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 100°C and 10⁻⁴ bar CO₂ Fugacity

Source: DTN: MO0304SPACSALT.000109c41/e.xls.xls

Figure B-09-6. Bin 09 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-4} bar CO_2 Fugacity

Source: OTN: MO0304SPACSAULT000009c217e.xls.xls

Figure B-09-7. Bin 09 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSA.LT.000:09c2f7e.xls.xls

Figure B-09-8. Bin 09 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 70°C and 10⁻² bar CO₂ Fugacity

Source: DTN: MO0304SPACSAIT.000009c3f7e.xls.xls

Figure B-09-10. Bin 09 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 70°C and 10–3 bar CO₂ Fugacity

Source: DTN: MO0304SPACSAIT 000V09c417a.xls.xls

Figure B-09-12. Bin 09 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\09c2t4e.xls.xls

Figure B-09-13. Bin 09 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\09c2t4e.xls.xls

Figure B-09-14. Bin 09 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\09c3t4e.xls.xls

Figure B-09-15. Bin 09 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\09c3t4e.xls.xls

Figure B-09-16. Bin 09 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\09c4t4e.xls.xls.

Figure B-9-17. Bin 09 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\09c4t4e.xls.xls.

Figure B-9-18. Bin 09 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\10c2t1e.xls.xls.

Figure B-10-1. Bin 10 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-2} bar CO_2 Fugacity

Sources: DTN: MO0304SPACSAULT.000\10c2t1e.xls.xls.

Figure B-10-2. Bin 10 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\10c3f1e.xls.xls

Figure B-10-3. Bin 10 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\10c3f1e.xls.xls

Figure B-10-4. Bin 10 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\10c4f1e.xls.xls

Figure B-10-5. Bin 10 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\10c4f1e.xls.xls

Figure B-10-6. Bin 10 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-4} bar CO_2 Fugacity

Figure B-10-7. Bin 10 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-2} bar CO_2 Fugacity

Figure B-10-9. Bin 10 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-3} bar CO_2 Fugacity

Figure B-10-8. Bin 10 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-2} bar CO_2 Fugacity

Figure B-10-10. Bin 10 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 70°C and 10⁻³ bar CO₂ Fugacity

Source: DTN: MO0304SPACSAULT.000A10c417e.xls.xls

Figure B-10-12. Bin 10 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 70°C and 10⁻⁴ bar CO₂ Fugacity

Source: DTN: MO0304SPACSAULT.000:10c214e.xls.xls

Figure B-10-14. Bin 10 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\10c3t4e.xls.xls.

Figure B-10-15. Bin 10 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\10c3t4e.xls.xls.

Figure B-10-16. Bin 10 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\10c4t4e.xls.xls.

Figure B-10-17. Bin 10 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\10c4t4e.xls.xls.

Figure B-10-18. Bin 10 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000A11c211e.xls.xls

Figure B-11-2. Bin 11 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000A11c31fe.xls.xls

Figure B-11-4. Bin 11 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\11c411e.xls.xls

Figure B-11-5. Bin 11 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\11c411e.xls.xls

Figure B-11-6. Bin 11 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\11c217e.xls.xls

Figure B-11-7. Bin 11 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSALT.000\11c217e.xls.xls

Figure B-11-8. Bin 11 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-2} bar CO_2 Fugacity

Figure 1 is a line graph showing the mobility of various ions in a polymer electrolyte membrane as a function of water uptake. The x-axis represents water uptake from 100% to 0%. The y-axis represents the mobility of ions on a logarithmic scale from 10^{-12} to 10^2 . The legend includes: S^{2-} , Br^- , Cl^- , ClO_4^- , NO_3^- , F^- , K^+ , Na^+ , Li^+ , H_2O , HCO_3^- , and pH. Mobility generally increases with water uptake, with S^{2-} showing the highest mobility and H_2O showing the lowest.

Figure 1 is a line graph showing the pH of various mineral solutions as a function of the mass ratio of mineral to glass. The x-axis represents the mass ratio from 100% to 0%, and the y-axis represents the pH from 3 to 12. The legend includes: H₂O (aq), Acetic acid, Carbonic acid, Phosphoric acid, Sulfuric acid, Nitric acid, Hydrofluoric acid, Hydrochloric acid, Sulfuric acid, Nitric acid, Hydrofluoric acid, Hydrochloric acid, and CH₃COOH (aq). The pH values generally decrease as the mass ratio of mineral to glass decreases, with some solutions showing a sharp drop in pH at specific ratios.

Source: DTN: MO0304SPACSAULT.000\11c3f7e.xls.xls

Source: DTN: MO0304SPACSA1T.000\11c307e.xls.xls

Source: DTN: MO0304SPACSAULT.000\11c214e.xls.xls.

Figure B-11-13. Bin 11 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\11c214e.xls.xls.

Figure B-11-14. Bin 11 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\11c314e.xls.xls.

Figure B-11-15. Bin 11 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000\11c314e.xls.xls.

Figure B-11-16. Bin 11 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0304SPACSAULT.000111c414e.xls.xls

Figure B-11-17. Bin 11 Aqueous Composition
Evaporation Predictions vs. Relative Humidity at
40°C and 10^{-4} bar CO_2 Fugacity

Source: DTN: MO6364SPACSAIT.000011/c4/4e.xls.xls

Figure B-11-18. Bin 11 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 40°C and 10⁻⁴ bar CO₂ Fugacity

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APPENDIX C
DUST LEACHATE LOOKUP TABLE RESULTS

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C. DUST LEACHATE LOOKUP TABLE RESULTS

The graphs presented in this document are representative of the information available in DTNs: MO0310SPADLALT.001 and MO0310SPADLHTL.000. Two graphs from each excel file shown here are: Aqueous Composition Evaporation Predictions vs. Relative Humidity, and Mineral Precipitation Evaporation Predictions vs. Relative Humidity. This information is provided for each respective bin and parameter setting. Also available in the respective excel files, but not shown here, are: ANC Species Concentration Evaporation Predictions vs. Relative Humidity, ANC Species Concentration Evaporation Predictions vs. Concentration Factor, Aqueous Composition Evaporation Predictions vs. Concentration Factor, and Mineral Precipitation Evaporation Predictions vs. Concentration.

The graphs given in this document are referenced only by the Bin number and parameter settings. Table C-1 gives the associated Excel source file name for the graphs in this document. Each excel file header contains the tractability back to the specific input data used in the calculation. The file nomenclature is *d?c#t%\$.xls*, where d represents the dust bin, "?" is the 1-digit bin number (1, 2, etc.), "#" is 2, 3, or 4 (for $p\text{CO}_2 = 10^{-\#}$), "%" is 04, 07, 10, 12, or 14 (for temp = 40°C, 70°C, 100°C, 120°C, or 140°C, respectively). FILE NAME EXAMPLE (*d1c2t10.xls*) is dust bin 1 at a $p\text{CO}_2$ of 10^{-2} at 100°C.

For the figures shown below, three terms need to be defined:

1. IS: Ionic Strength
2. RH: Relative Humidity
3. a(w) = Activity of Water.

The values in Table C-2 correspond to the given parameters extracted from the excel files in DTNs: MO0310SPADLALT.001 and MO0310SPADLHTL.000. Given in this table are deliquescence point relative humidity and the associated chemical parameters of interest to the TSPA.

Table C-1. Excel File Names for Each Lookup Table

Bin	Look-up Tables
1	d1c2t04.xls, d1c3t04.xls, d1c4t04.xls, d1c2t07.xls, d1c3t07.xls, d1c4t07.xls, d1c2t10.xls, d1c3t10.xls, d1c4t10.xls, d1c2t12.xls, d1c3t12.xls, d1c4t12.xls, d1c2t14.xls, d1c3t14.xls, d1c4t14.xls
2	d2c2t04.xls, d2c3t04.xls, d2c4t04.xls, d2c2t07.xls, d2c3t07.xls, d2c4t07.xls, d2c2t10.xls, d2c3t10.xls, d2c4t10.xls, d2c2t12.xls, d2c3t12.xls, d2c4t12.xls, d2c2t14.xls, d2c3t14.xls, d2c4t14.xls
3	d3c2t04.xls, d3c3t04.xls, d3c4t04.xls, d3c2t07.xls, d3c3t07.xls, d3c4t07.xls, d3c2t10.xls, d3c3t10.xls, d3c4t10.xls, d3c2t12.xls, d3c3t12.xls, d3c4t12.xls, d3c2t14.xls, d3c3t14.xls, d3c4t14.xls
4	d4c2t04.xls, d4c3t04.xls, d4c4t04.xls, d4c2t07.xls, d4c3t07.xls, d4c4t07.xls, d4c2t10.xls, d4c3t10.xls, d4c4t10.xls, d4c2t12.xls, d4c3t12.xls, d4c4t12.xls, d4c2t14.xls, d4c3t14.xls, d4c4t14.xls
5	d5c2t04.xls, d5c3t04.xls, d5c4t04.xls, d5c2t07.xls, d5c3t07.xls, d5c4t07.xls, d5c2t10.xls, d5c3t10.xls, d5c4t10.xls, d5c2t12.xls, d5c3t12.xls, d5c4t12.xls, d5c2t14.xls, d5c3t14.xls, d5c4t14.xls
6	d6c2t04.xls, d6c3t04.xls, d6c4t04.xls, d6c2t07.xls, d6c3t07.xls, d6c4t07.xls, d6c2t10.xls, d6c3t10.xls, d6c4t10.xls, d6c2t12.xls, d6c3t12.xls, d6c4t12.xls, d6c2t14.xls, d6c3t14.xls, d6c4t14.xls

Source: DTNs: MO0310SPADLALT.001 (for 40°C, 70°C, and 100°C) and MO0310SPADLHTL.000 (for 120°C and 140°C).

Table C-2. Deliquescence Point Relative Humidity and Associated Chemical Parameters Taken from the Dust Leachate Lookup Tables

Bin	Temperature (Celsius)	$p\text{CO}_2$ (bars)	Deliquescence Point Relative Humidity	pH	Ionic Strength (Moles/kg. H_2O)	Cl (Moles/kg. H_2O)	NO_3 (Moles/kg. H_2O)
1	40	0.0100	50.0%	6.896	1.541E+01	4.269E+00	5.921E+00
	70		30.0%	9.106	4.17E+01	1.04E-01	2.78E+01
	100		31.5%	8.780	4.219E+01	1.306E-01	2.837E+01
	120		30.8%	6.486	2.782E+01	1.065E+00	2.089E+01
	140		26.2%	6.255	2.780E+01	5.061E-01	2.552E+01
	40	0.0010	50.0%	7.402	1.541E+01	4.262E+00	5.912E+00
	70		30.0%	9.612	4.178E+01	1.027E-01	2.782E+01
	100		31.5%	9.286	4.227E+01	1.294E-01	2.842E+01
	120		30.7%	6.801	2.732E+01	1.031E+00	2.199E+01
	140		26.2%	6.752	2.782E+01	5.078E-01	2.554E+01
	40	0.0001	50.0%	7.903	1.541E+01	4.261E+00	5.908E+00
	70		30.0%	10.110	4.178E+01	1.030E-01	2.782E+01
	100		32.4%	9.318	3.715E+01	2.727E-01	2.490E+01
	120		30.8%	7.454	2.782E+01	1.066E+00	2.106E+01
	140		26.2%	7.253	2.783E+01	5.038E-01	2.557E+01
2	40	0.0100	58.1%	7.135	1.181E+01	2.404E+00	3.881E+00
	70		47.8%	7.763	1.918E+01	1.306E+00	1.423E+01
	100		42.2%	7.984	2.108E+01	1.893E+00	1.524E+01
	120		35.4%	7.929	2.869E+01	3.784E+00	1.656E+01
	140		32.0%	8.369	2.406E+01	2.088E+00	1.827E+01
	40	0.0010	58.1%	7.635	1.181E+01	2.404E+00	3.881E+00
	70		47.8%	8.263	1.918E+01	1.306E+00	1.423E+01
	100		42.2%	8.484	2.108E+01	1.893E+00	1.524E+01
	120		35.4%	8.445	2.840E+01	3.752E+00	1.655E+01
	140		32.0%	8.869	2.406E+01	2.088E+00	1.827E+01
	40	0.0001	58.1%	8.135	1.181E+01	2.404E+00	3.882E+00
	70		47.8%	8.763	1.918E+01	1.306E+00	1.423E+01
	100		42.2%	8.984	2.108E+01	1.893E+00	1.524E+01
	120		35.4%	8.947	2.836E+01	3.749E+00	1.654E+01
	140		32.0%	9.369	2.406E+01	2.088E+00	1.827E+01

Table C-2. Deliquescence Point Relative Humidity and Associated Chemical Parameters Taken from the Dust Leachate Lookup Tables (Continued)

Bin	Temperature (Celsius)	$p\text{CO}_2$ (bars)	Deliquescence Point Relative Humidity	pH	Ionic Strength (Moles/kg. H_2O)	Cl (Moles/kg. H_2O)	NO_3 (Moles/kg. H_2O)
3	40	0.0100	60.5%	9.802	1.683E+01	1.857E+00	1.469E+01
	70		49.9%	10.121	1.866E+01	2.207E+00	1.151E+01
	100		42.8%	10.768	2.408E+01	2.265E+00	1.521E+01
	120		38.4%	10.544	2.332E+01	2.343E+00	1.821E+01
	140		32.4%	10.717	2.810E+01	1.554E+00	1.986E+01
	40	0.0010	58.8%	10.125	1.351E+01	3.128E+00	3.618E+00
	70		50.0%	10.685	1.870E+01	2.235E+00	1.146E+01
	100		43.2%	11.237	2.376E+01	2.425E+00	1.525E+01
	120		38.5%	11.027	2.313E+01	2.418E+00	1.821E+01
	140		32.6%	11.152	2.732E+01	1.732E+00	1.995E+01
	40	0.0001	58.8%	10.714	1.360E+01	3.181E+00	3.508E+00
	70		50.0%	11.180	1.866E+01	2.253E+00	1.145E+01
	100		43.4%	11.731	2.365E+01	2.469E+00	1.525E+01
	120		38.6%	11.519	2.307E+01	2.451E+00	1.822E+01
	140		32.6%	11.644	2.707E+01	1.758E+00	1.992E+01
4	40	0.0100	52.9%	7.195	1.343E+01	1.288E+00	5.884E+00
	70		45.4%	7.850	2.082E+01	7.776E-01	1.620E+01
	100		36.4%	8.286	2.481E+01	5.950E-01	2.172E+01
	120		31.2%	8.518	2.646E+01	5.313E-01	2.384E+01
	140		26.4%	8.680	2.794E+01	4.657E-01	2.574E+01
	40	0.0010	52.9%	7.695	1.343E+01	1.288E+00	5.886E+00
	70		44.5%	8.422	2.123E+01	8.213E-01	1.727E+01
	100		36.4%	8.786	2.481E+01	5.950E-01	2.172E+01
	120		31.2%	9.018	2.646E+01	5.314E-01	2.384E+01
	140		26.4%	9.180	2.794E+01	4.658E-01	2.574E+01
	40	0.0001	52.9%	8.195	1.343E+01	1.288E+00	5.887E+00
	70		44.5%	8.922	2.123E+01	8.213E-01	1.727E+01
	100		36.4%	9.286	2.481E+01	5.950E-01	2.172E+01
	120		31.2%	9.518	2.646E+01	5.314E-01	2.384E+01
	140		26.4%	9.680	2.794E+01	4.658E-01	2.574E+01

Table C-2. Deliquescence Point Relative Humidity and Associated Chemical Parameters Taken from the Dust Leachate Lookup Tables (Continued)

Bin	Temperature (Celsius)	$p\text{CO}_2$ (bars)	Deliquescence Point Relative Humidity	pH	Ionic Strength (Moles/kg. H_2O)	Cl (Moles/kg. H_2O)	NO_3 (Moles/kg. H_2O)
5	40	0.0100	56.1%	7.787	1.307E+01	1.867E+00	4.724E+00
	70		45.2%	8.448	2.171E+01	7.877E-01	1.646E+01
	100		41.8%	8.374	2.728E+01	2.307E+00	1.709E+01
	120		31.1%	8.904	2.709E+01	5.534E-01	2.392E+01
	140		26.3%	9.031	2.836E+01	4.801E-01	2.576E+01
	40	0.0010	56.1%	8.286	1.307E+01	1.868E+00	4.725E+00
	70		45.2%	8.948	2.171E+01	7.878E-01	1.646E+01
	100		41.8%	8.870	2.736E+01	2.315E+00	1.709E+01
	120		31.1%	9.403	2.709E+01	5.536E-01	2.392E+01
	140		26.3%	9.531	2.836E+01	4.803E-01	2.576E+01
	40	0.0001	56.1%	8.786	1.307E+01	1.868E+00	4.725E+00
	70		45.2%	9.448	2.171E+01	7.879E-01	1.646E+01
	100		41.8%	9.374	2.725E+01	2.307E+00	1.708E+01
	120		31.1%	9.903	2.709E+01	5.536E-01	2.392E+01
	140		26.3%	10.030	2.836E+01	4.804E-01	2.576E+01
6	40	0.0100	59.8%	9.139	1.262E+01	3.751E+00	3.274E+00
	70		55.9%	10.203	1.768E+01	4.049E+00	1.126E+01
	100		42.8%	10.767	2.409E+01	2.268E+00	1.521E+01
	120		38.4%	10.542	2.333E+01	2.351E+00	1.822E+01
	140		32.3%	10.654	2.830E+01	1.701E+00	2.020E+01
	40	0.0010	59.4%	10.124	1.304E+01	3.676E+00	3.226E+00
	70		49.7%	10.952	2.074E+01	2.687E+00	9.194E+00
	100		43.2%	11.233	2.377E+01	2.436E+00	1.525E+01
	120		38.5%	10.118	1.906E+01	6.655E+00	2.718E+00
	140		32.6%	11.215	2.717E+01	1.575E+00	1.959E+01
	40	0.0001	59.3%	10.714	1.329E+01	3.644E+00	3.190E+00
	70		49.4%	11.469	2.102E+01	2.693E+00	9.262E+00
	100		43.4%	11.724	2.366E+01	2.487E+00	1.525E+01
	120		38.6%	11.518	2.307E+01	2.456E+00	1.822E+01
	140		32.7%	11.683	2.697E+01	1.658E+00	1.970E+01

Source: DTNs: MO0310SPADLALT.001 (for 40°C, 70°C, and 100°C) and MO0310SPADLHTL.000 (for 120°C and 140°C).

Source: DTN: MO03104SPADLALT.001\dfc2104.xls

Figure C-01-2. Bin 01 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPADLALT.000\dt1c2107.xls

Figure C-01-4. Bin 01 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0310SPADLALT.001\dlc2t10.xls

Figure C-01-5. Bin 01 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0310SPADLHTL.000\dlc2t12.xls

Figure C-01-7. Bin 01 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 120°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0304SPADLALT.000\dlc2t10.xls

Figure C-01-6. Bin 01 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0310SPADLHTL.000\dlc2t12.xls

Figure C-01-8. Bin 01 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 120°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0310SPADLHTL.000\dlc2t114.xls.

Figure C-01-9. Bin 01 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 140°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO03010SPADLALT.001\dlc3t04.xls.

Figure C-01-11. Bin 01 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0310SPADLHTL.000\dlc2t114.xls.

Figure C-01-10. Bin 01 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 140°C and 10^{-2} bar CO_2 Fugacity

Source: DTN: MO0310SPADLALT.001\dlc3t04.xls.

Figure C-01-12. Bin 01 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 40°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0310SPADLALT.001\dlc3i07.xls.

Figure C-01-13. Bin 01 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0310SPADLALT.001\dlc3i10.xls.

Figure C-01-15. Bin 01 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0310SPADLALT.001\dlc3i07.xls.

Figure C-01-14. Bin 01 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 70°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0310SPADLALT.001\dlc3i10.xls.

Figure C-01-16. Bin 01 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 100°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: \MO0310SPADLHTL.000\dfc3f12.xls.

Figure C-01-17. Bin 01 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 120°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0310SPADLHTL.000\dfc3f14.xls.

Figure C-01-19. Bin 01 Aqueous Composition Evaporation Predictions vs. Relative Humidity at 140°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0310SPADLHTL.000\dfc3f12.xls.

Figure C-01-18. Bin 01 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 120°C and 10^{-3} bar CO_2 Fugacity

Source: DTN: MO0310SPADLHTL.000\dfc3f14.xls.

Figure C-01-20. Bin 01 Mineral Precipitation Evaporation Predictions vs. Relative Humidity at 140°C and 10^{-3} bar CO_2 Fugacity