OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
ANALYSIS/MODEL COVER SHEET

1. QA: QA

Complete Only Applicable Items

2. ☐ Analysis	Check all that apply	3. ☒ Model	Check all that apply
Type of Analysis	☐ Engineering ☐ Performance Assessment ☐ Scientific	Type of Model	☒ Conceptual Model ☒ Abstraction Model ☐ Mathematical Model ☐ System Model ☐ Process Model
Intended Use of Analysis	☐ Input to Calculation ☐ Input to another Analysis or Model ☐ Input to Technical Document ☐ Input to other Technical Products	Intended Use of Model	☐ Input to Calculation ☒ Input to another Model or Analysis ☐ Input to Technical Document ☐ Input to other Technical Products
Describe use:		Describe use:	The use of this conceptual model is to provide qualitative explanations of interrelationships among models in the input AMRs in order to clarify general guidance to TSPA.

4. Title:
Physical and Chemical Environmental Abstraction Model

5. Document Identifier (including Rev. No. and Change No., if applicable):
ANL-EBS-MD-000046 REV 00

6. Total Attachments:

7. Attachment Numbers - No. of Pages in Each:
I-3

		Printed Name	Signature	Date
8.	Originator	E. James Nowak	Robert MacKinnon for EN	4/14/00
9.	Checker (Technical)	Hans Papenguth	Robert MacKinnon for HP	4/14/00
	Checker (Compliance)	Leland C. Powell	L C Powell	4-14-00
10.	Lead/Supervisor	Robert MacKinnon	Robert MacKinnon	4/14/00
11.	Responsible Manager	Robert MacKinnon	Robert MacKinnon	4/14/00

12. Remarks:

Enclosure 1

NM5507

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
ANALYSIS/MODEL REVISION RECORD
Complete Only Applicable Items

2. Analysis or Model Title:

Physical and Chemical Environmental Abstraction Model

3. Document Identifier (including Rev. No. and Change No., if applicable):

ANL-EBS-MD-000046 REV 00

4. Revision/Change No.	5. Description of Revision/Change
00	Initial Issue

DISCLAIMER

This contractor document was prepared for the U.S. Department of Energy (DOE), but has not undergone programmatic, policy, or publication review, and is provided for information only. The document provides preliminary information that may change based on new information or analysis, and represents a conservative treatment of parameters and assumptions to be used specifically for Total System Performance Assessment analyses. The document is a preliminary lower level contractor document and is not intended for publication or wide distribution.

Although this document has undergone technical reviews at the contractor organization, it has not undergone a DOE policy review. Therefore, the views and opinions of authors expressed may not state or reflect those of the DOE. However, in the interest of the rapid transfer of information, we are providing this document for your information per your request.

CONTENTS

Page

FIGURES

Page

TABLES

Page

1. PURPOSE

As directed by a written development plan (CRWMS M&O 1999a), Task 1, an overall conceptualization of the physical and chemical environment (P/CE) in the emplacement drift is developed in this Analysis/Model Report (AMR). Included in the model are the physical components of the engineered barrier system (EBS). The purpose of this conceptual model is to assist Performance Assessment Operations (PAO) and its Engineered Barrier Performance Section in modeling the physical and chemical environment within a repository drift, thus allowing PAO to provide a more integrated and complete in-drift geochemical model abstraction and to answer the key technical issues raised in the U.S. Nuclear Regulatory Commission (NRC) Issue Resolution Status Report (IRSR) for the Evolution of the Near-Field Environment (NFE) Revision 2 (NRC 1999). EBS-related features, events, and processes (FEPs) have been assembled and discussed in *EBS FEPs/Degradation Modes Abstraction* (CRWMS M&O 2000a). Input AMRs listed in Section 4.1 FEPs address that have not been screened out. This AMR does not directly address those FEPs. Additional tasks described in the written development plan are recommended for future work in Section 7.3.

To achieve the stated purpose, the scope of this document includes:

- the role of in-drift physical and chemical environments in the Total System Performance Assessment (TSPA) (Section 6.1);
- the configuration of engineered components (features) and critical locations in drifts (Sections 6.2.1 and 6.3, portions taken from *EBS Radionuclide Transport Abstraction* (CRWMS M&O 2000b));
- overview and critical locations of processes that can affect P/CE (Section 6.3);
- couplings and relationships among features and processes in the drifts (Section 6.4);
- identities and uses of parameters transmitted to TSPA in sub-model AMRs (Section 6.5); and
- directions for use of the conceptual model and sub-model parameters in subsequent PAO abstractions and analyses (Section 6.5).

The intended use of this conceptual model is to provide qualitative explanations of interrelationships among models in the input AMRs in order to clarify general guidance to TSPA.

This model has been developed to serve as an explanatory basis for the in-drift physical and chemical analyses performed by PAO.

2. QUALITY ASSURANCE

The Quality Assurance (QA) program applies to the development of this conceptual model documentation. The Performance Assessment Operations responsible manager has evaluated the technical document development activity in accordance with QAP-2-0 activity evaluation, *Conduct of Activities.* The QAP-2-0 activity evaluation, *Conduct of Performance Assessment* (CRWMS M&O 1999b), has determined that the preparation and review of this technical document is subject *Quality Assurance Requirements and Description* (QARD) DOE/RW-0333P (DOE 2000) requirements. Preparation of this analysis did not require the classification of items in accordance with QAP-2-3, *Classification of Permanent Items.* This activity is not a field activity. Therefore an evaluation in accordance with NLP-2-0, *Determination of Importance Evaluations* was not required.

3. COMPUTER SOFTWARE AND MODEL USAGE

3.1 COMPUTER SOFTWARE

No codes, routines, or software were developed or used for this conceptual model.

3.2 MODELS

The previous model use of the PAO in-drift physical and chemical environment analysis is documented in Chapter 4 of the *Total System Performance Assessment-Viability Assessment (TSPA-VA) Analyses Technical Basis Document* (CRWMS M&O 1998). This conceptual model document is being developed to supercede the concepts presented in the Technical Basis Document.

4. INPUTS

4.1 DATA AND PARAMETERS

No input data and parameters were used to develop the conceptual model documented in this report.

4.2 CRITERIA

Programmatic requirements for this document are listed in the Development Plan *Physical and Chemical Environment Model for TSPA-LA* (CRWMS M&O 1999a). That Development Plan specifies that this document and all analyses described herein must adhere to the requirements of AP-3.10Q, *Analyses and Models,*and must address applicable NRC issue resolution status report (IRSR) criteria (NRC 1999).

Below is a summary of the applicable NRC review methods and acceptance criteria outlined in the Issue Resolution Status Report (IRSR) that apply to model development for the following near-field environment key technical issue sub-issue effects: (a) coupled thermal-hydrologic-chemical processes on the waste package chemical environment, (b) coupled thermal-hydrologic-chemical (THC) processes on the chemical environment for radionuclide release, and (c) coupled THC processes on radionuclide transport through engineered and natural barriers (NRC 1999). Also included below is a listing of the project features, events, and processes (FEPs) that apply to this report.

4.2.1 NRC IRSR Criteria

Evaluations of the criteria are discussed in Section 7.2.

4.2.1.1 Data and Model Justification Acceptance Criteria

1. Consider both temporal and spatial variations in THC effects on the chemical environment for radionuclide release. (NRC 1999, Sections 4.1.1, 4.2.1, 4.3.1, and 4.4.1)

2. Consider site characteristics in establishing initial and boundary conditions for conceptual models and simulations of coupled processes that may affect the chemical environment for radionuclide release. (NRC 1999, Sections 4.1.1, 4.2.1, 4.3.1, and 4.4.1)

3. Collect sufficient data on the characteristics of the natural system and engineered materials, such as the type, quantity, and reactivity of materials, in establishing initial and boundary conditions for conceptual models and simulations of THC coupled processes that may affect the chemical environment for radionuclide release. (NRC 1999, Sections 4.1.1, 4.2.1, 4.3.1, and 4.4.1)

4. Use sensitivity and uncertainty analyses (including consideration of alternative conceptual models) to determine whether additional new data are needed to better define ranges of input parameters. (NRC 1999, Sections 4.1.1, 4.2.1, 4.3.1, and 4.4.1)

5. If the testing program for coupled THC processes on the chemical environment for radionuclide release from the engineered barrier system is not complete at the time of license application, or if sensitivity and uncertainty analyses indicate that additional data are needed, identify specific plans to acquire the necessary information as part of the performance confirmation program. (NRC 1999, Sections 4.1.1, 4.2.1, 4.3.1, and 4.4.1)

4.2.1.2 Data Uncertainty and Verification Acceptance Criteria

1. Use reasonable or conservative ranges of parameters or functional relations to determine effects of coupled THC processes on the chemical environment for radionuclide release. Parameter values, assumed ranges, probability distributions, and bounding assumptions should be technically defensible and reasonably account for uncertainties. (NRC 1999, Sections 4.1.1, 4.2.1, 4.3.1, and 4.4.1)

2. Consider uncertainty in data due to both temporal and spatial variations in conditions affecting coupled THC effects on the chemical environment for radionuclide release. (NRC 1999, Sections 4.1.1, 4.2.1, 4.3.1, and 4.4.1)

3. Properly consider the uncertainties in the characteristics of the natural system and engineered materials when evaluating coupled THC processes. Among those uncertainties are the type, quantity, and reactivity of materials, in establishing initial and boundary conditions for conceptual models and simulations of THC coupled processes that may affect the chemical environment for radionuclide release. (NRC 1999, Sections 4.1.1, 4.2.1, 4.3.1, and 4.4.1)

4. The initial conditions, boundary conditions, and computational domain used in sensitivity analysis involving coupled THC effects on the chemical environment for radionuclide release should be consistent with available data. (NRC 1999, Sections 4.1.1, 4.2.1, 4.3.1, and 4.4.1)

5. DOE's performance confirmation program should assess whether the natural system and engineered materials are functioning as intended and anticipated with regard to coupled THC effects on the chemical environment for radionuclide release from the engineered barrier system (EBS). (NRC 1999, Sections 4.1.1, 4.2.1, 4.3.1, and 4.4.1)

4.2.1.3 Model Uncertainty Acceptance Criteria

1. Use appropriate models, tests, and analyses that are sensitive to the THC couplings under consideration for both natural and engineered systems as described in the following examples. The effects of THC coupled processes that may occur in the natural setting or due to interactions with engineered materials or their alteration products include: (i) thermohydrologic (TH) effects on gas and water chemistry; (ii) hydrothermally driven geochemical reactions, such as zeolitization of volcanic glass; (iii) dehydration of hydrous phases liberating moisture; (iv) effects of microbial processes; and (v) changes in water chemistry that may result from interactions between cementitious or waste package materials and groundwater, which, in turn, may affect the chemical environment for radionuclide release. (NRC 1999, Sections 4.1.1, 4.2.1, 4.3.1, and 4.4.1)

2. Investigate alternative modeling approaches consistent with available data and current scientific understanding, and appropriately consider the modeling results and limitations. (NRC 1999, Sections 4.1.1, 4.2.1, 4.3.1, and 4.4.1)

3. Provide a reasonable description of the mathematical models included in analyses of coupled THC effects on the chemical environment for radionuclide release. The description should include a discussion of alternative modeling approaches not considered in the final analysis and the limitations and uncertainties of the chosen model. (NRC 1999, Sections 4.1.1, 4.2.1, 4.3.1, and 4.4.1)

4.2.1.4 Model Verification Acceptance Criteria

1. The mathematical models for coupled THC effects on the chemical environment for radionuclide release should be consistent with conceptual models based on inferences about the near-field environment, field data and natural alteration observed at the site, and expected engineered materials. (NRC 1999, Sections 4.1.1, 4.2.1, 4.3.1, and 4.4.1)

2. Appropriately adopt accepted and well-documented procedures to construct and test the numerical models used to simulate coupled THC effects on the chemical environment for radionuclide release. (NRC 1999, Sections 4.1.1, 4.2.1, 4.3.1, and 4.4.1)

3. Abstracted models for coupled THC effects on the chemical environment for radionuclide release should be based on the same assumptions and approximations shown to be appropriate for closely analogous natural or experimental systems. Abstracted model results should be verified by comparison with outputs of detailed process models and empirical observations. Abstracted model results should be compared with different mathematical models to judge robustness of results. (NRC 1999, Sections 4.1.1, 4.2.1, 4.3.1, and 4.4.1)

4.2.2 YMP Features, Events, and Processes (FEPs)

A list of the FEPs that could affect the performance of the repository has been assembled and discussed in *EBS FEPs/Degradation Modes Abstraction* (CRWMS M&O 2000a). Input AMRs listed in Section 6.0 address FEPs that have not been screened out. This AMR does not directly address those FEPs.

4.3 CODES AND STANDARDS

4.3.1 Codes

No codes were used in this document.

4.3.2 Standards

No standards were used in this document.

5. ASSUMPTIONS

No assumptions are inherent in the development of this model.

6. ANALYSIS/MODEL

The conceptual model developed in this AMR and to be implemented in other document(s) that will be developed improves upon and supersedes the previous model used in TSPA-VA in-drift geochemical analyses (CRWMS M&O 1998).

The intended use of this conceptual model is to provide qualitative explanations of the interrelationships and integration among sub-models in the resource AMRs. It is a model in which validated sub-models become an integrated whole. In that sense, it is a model abstraction. The validity of this model for that intended use is derived in part from validity of the conceptual models in the input AMRs, which provide scientific bases for the integrated whole. Validity is also derived from the straightforward use of the scientific principle of conservation of mass in that fluid constituents leaving the domain of one sub-model along transport paths defined by *EBS Radionuclide Transport Abstraction* (CRWMS M&O 2000b) arrive in the next sub-model domain along the path. That level of model validation is adequate for the intended use.

Several conceptual models and sub-models from other AMRs were used as resources for the development of the conceptual model of the in-drift P/CE given in this AMR. A list of resource AMRs follows:

- *EBS FEPs/Degradation Modes Abstraction* (CRWMS M&O 2000a)
- *EBS Radionuclide Transport Abstraction* (CRWMS M&O 2000b)
- *Abstraction of Drift-Scale Coupled Processes* (CRWMS M&O 2000c)
- *Develop the In-Package Chemistry Abstraction for TSPA-LA* (CRWMS M&O 2000d)
- *In-Drift Microbial Communities* (CRWMS M&O 2000e)
- *In-Drift Gas Flux and Composition* (CRWMS M&O 2000f)
- *Miscellaneous Waste Form FEPs Screening Argument* (CRWMS M&O 2000g)
- *Seepage/Cement Interactions* (CRWMS M&O 2000h)
- *Seepage/Invert Interactions* (CRWMS M&O 2000i)
- *In-Drifts Precipitates/Salts Analysis* (CRWMS M&O 2000j)
- *FEPs Screening of Processes and Issues in Drip Shield and Waste Package Degradation* (CRWMS M&O 2000k)
- *Colloid-Associated Concentration Limits-Abstraction and Summary* (CRWMS M&O 2000l)
- *Seepage/Backfill Interactions* (CRWMS M&O 2000m)
- *In-Drift Colloids and Concentrations* (CRWMS M&O 2000n)
- *Abstraction of NFE Drift Thermodynamic Environment and Percolation Flux* (CRWMS M&O 2000o)

6.1 THE ROLE OF IN-DRIFT PHYSICAL AND CHEMICAL ENVIRONMENTS IN THE TSPA

The role of the P/CE conceptual model developed in this AMR, combined with models and analyses reported in resource AMRs listed above, is in describing in-drift transport and calculating the changes in water chemistry resulting from the interaction of introduced materials with water in the drift (CRWMS M&O 1999a). Potential factors affecting the environments are the temporal (a) evolution of groundwater flow paths in the drift and to the unsaturated zone of the host rock, and (b) composition of groundwater moving along those paths. Physical characteristics are needed to quantify groundwater movements in the drift that transport radioactive materials into the unsaturated zone. Brine composition values are needed to predict breaching of metallic engineered barriers by corrosion and to quantify processes that release and transport material from the waste forms to and through the host rock.

6.2 GENERAL IN-DRIFT DESIGN, INITIAL CONDITIONS, AND BOUNDARY CONDITIONS

6.2.1 In-Drift General Design Features

Figure 1 (CRWMS M&O 2000b) shows general design features of waste disposal drifts that affect the physical environment in which waste materials may be mobilized and transported into the unsaturated zone of the host rock. Waste forms are contained in metal waste packages. These packages lie on supports that rest on a flat invert composed of crushed host rock, with steel and copper components. A titanium alloy drip shield, resting on the invert, covers the waste package and pedestal. Drip shields are intended to divert entering groundwater from contact with waste packages. Eventually some drip shields will be penetrated by gaps and cease to shield the packages from groundwater. Backfill, consisting of sand (CRWMS M&O 2000m), may initially fill most of the drifts outside the drip shields, leaving an air gap near the tops of the drifts.

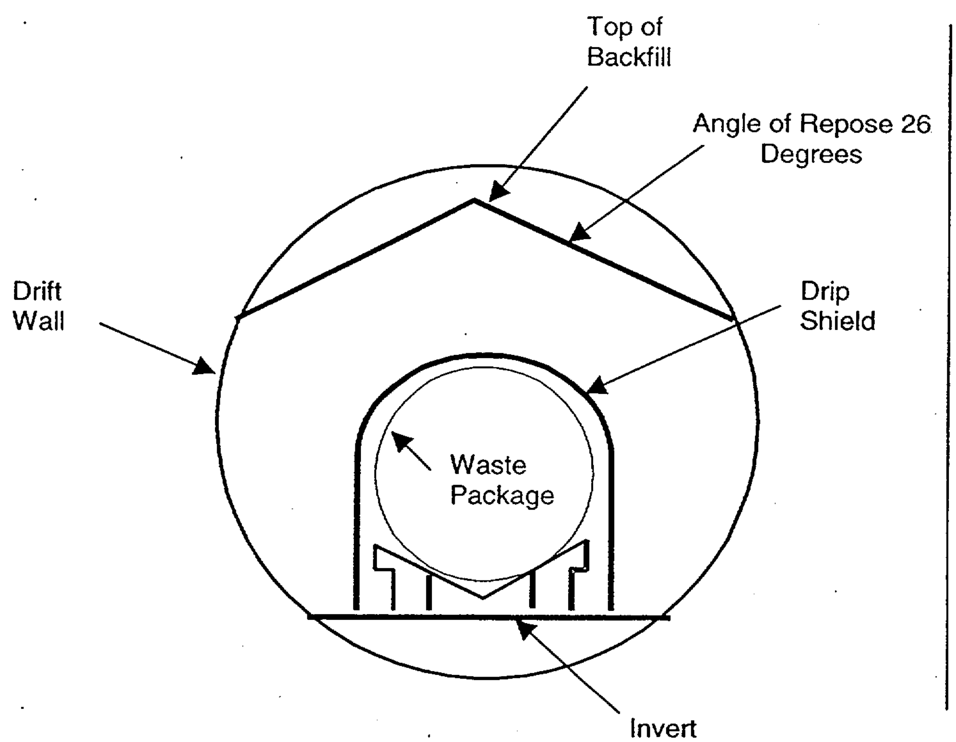

Figure 1. Schematic Diagram of a Typical Emplacement Drift and the Major Components of the EBS (adapted from *EBS Radionuclide Transport Abstraction* CRWMS M&O (2000b)).

6.2.2 Initial and Boundary Conditions

The thermal-hydrologic-chemistry (THC) effects on water chemistry and gas-phase composition adjacent to the drift wall in the near field host rock, the physical boundary of the drift, are abstracted in *Abstraction of Drift-Scale Coupled Processes* (CRWMS M&O 2000c). The process-level thermal hydrology (TH) model that characterizes the in-drift thermodynamic environment is abstracted in *Abstraction of NFE Drift Thermodynamic Environment and Percolation Flux* (CRWMS M&O 2000o).

6.3 OVERVIEW AND CRITICAL LOCATIONS OF PROCESSES THAT CAN AFFECT P/CE

Several processes potentially affect the in-drift environment that is relevant to performance assessment. This overview describes those processes and their interrelationships, although results from input AMRs and other documents may show that some of them can be neglected. Groundwater flow and transport, in *EBS Radionuclide Transport Abstraction* (CRWMS M&O 2000b), serve to define critical locations for the chemical processes (e.g., evaporation, precipitation, dissolution, and corrosion) and show how materials move among the locations. Chemical processes are treated and modeled at the critical locations.

Groundwater flow and transport are analyzed and modeled in *EBS Radionuclide Transport Abstraction* (CRWMS M&O 2000b). Figure 2, adapted from that AMR, shows the important flow pathways (arrows) for transport. The critical locations identified in Figure 2 are where the important in-drift processes occur and are modeled. Those locations are where groundwater compositions may change (to concentrated brines in some instances) due to evaporation, precipitation, redissolution, mixing, dilution, reactions with ambient gases, and other chemical reactions such as corrosion and waste form dissolution. Barriers are breached, radionuclides are mobilized, radionuclide species are formed, and groundwater steams are diverted and may also mix at those locations. Those processes are analyzed and modeled in the resource AMRs listed in Section 6.

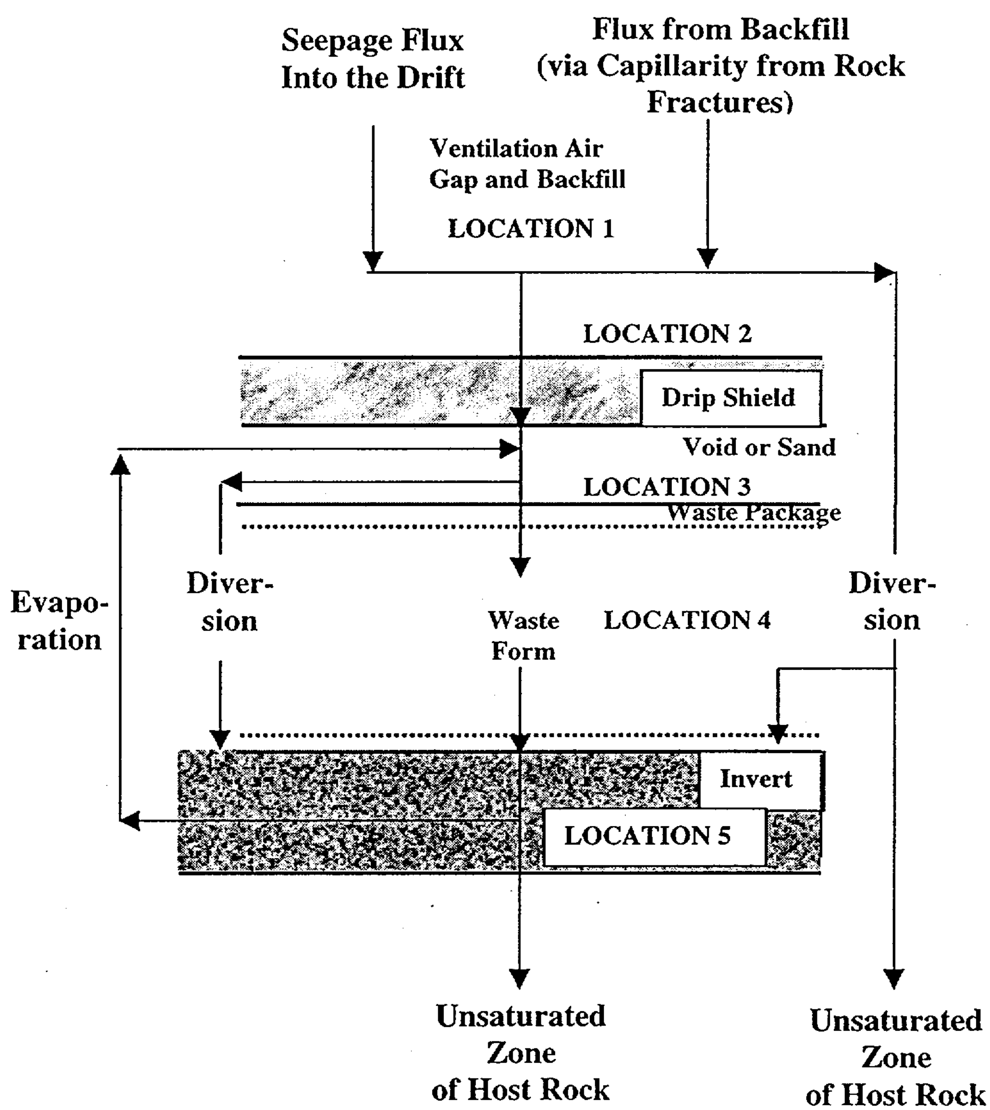

Figure 2. Structure Of EBS Flow and Transport Model with flow pathways (arrows) and critical locations shown (taken from *EBS Radionuclide Transport Abstraction* (CRWMS M&O 2000b)).

When temperatures at drift surfaces decrease sufficiently, seepage water enters the drift by gravity (by dripping) and capillary flux. Seepage drips through the air gap above the backfill and then through the backfill. Capillary fluxes of groundwater also pass through the backfill. The air gap and backfill are in LOCATION 1. Reactions with ambient gases, evaporation, salt precipitation, and salt redissolution to form groundwater brines occur there. The surface of the drip shield, LOCATION 2, is where groundwater is diverted and evaporation of groundwater, salt precipitation, brine formation, and breaching occur. The drip shield diverts groundwater fluxes which may pass through the invert to the UZ or may enter the UZ directly, potentially through backfill. Mechanically induced gaps and corrosion may breach the drip shield. Groundwater then can pass through breaches in the drip shield and contact the surface of the waste package at LOCATION 3, where it is diverted to the invert until the waste package is breached. That portion of groundwater that passes through breaches in the waste package will contact the waste forms at LOCATION 4. Groundwater flow and (and possibly molecular diffusion when advection does not dominate transport) carry radionuclide-containing species from waste forms inside the waste package to the invert, LOCATION 5. Three streams may pass through the invert to the unsaturated zone of the host rock: They come directly from the waste form and from diversion by the drip shield and waste package. Water diverted by the drip shield may enter the UZ through backfill if backfill is present. Transport to the unsaturated zone may also occur by molecular diffusion (also in LOCATION 5) when advection does not dominate transport.

Groundwater flow and transport and chemical processes can be summarized as follows:

- LOCATION 1: Ventilation Air Gap and Backfill. Seepage and capillary fluxes of groundwater. Chemical interactions among groundwater, cementitious grout around rock bolts, drift gases, and sand backfill. Also evaporation, condensation, salt precipitation, redissolution of salt, groundwater brine formation, and corrosion of the drip shield.

- LOCATION 2: Drip shield surface. Groundwater flow split to invert, host rock, and waste package. Corrosion of drip shield by groundwater/brine formed at location 1.

- LOCATION 3: Waste package surface. Groundwater flow split to invert and waste form. Evaporation, condensation, salt precipitation, redissolution of salt, interaction with ambient gases, groundwater brine formation, and corrosion of the waste package.

- LOCATION 4: Waste form. Groundwater flow and molecular diffusion from waste form to invert. Interaction with ambient gases, waste form dissolution, and other chemical processes that alter groundwater composition and mobilize radionuclide-containing species.

- LOCATION 5. Invert. Potential groundwater mixing, and transport by advection and molecular diffusion (if advection does not dominate transport) to unsaturated zone of host rock. Chemical interactions among (a) groundwaters, (b) drift gases and (c) crushed host rock invert material. Also evaporation, condensation, salt precipitation, redissolution of salt, groundwater brine formation, and corrosion of steel support materials. Here, groundwater compositions, groundwater mixing, solubilities, and colloid stabilities may determine the final composition of groundwater entering the unsaturated zone.

6.4 INTEGRATED PERFORMANCE-RELATED IN-DRIFT FEATURES AND PROCESSES CONSISTENT WITH SCREENED-IN FEPS AND INPUT AMRS

This section gives more detailed descriptions of the processes given in the overview of Section 6.3. LOCATIONS are shown in Figure 2 of Section 6.3. These processes potentially affect the in-drift environment. Although included here, results from resource AMRs and other documents may show that some of them can be neglected.

The descriptions in the following subsections generally summarize and explain interrelationships among conceptual models from the resource AMRs that are cited after each subsection. Most subsections draw from the following AMRs:

EBS Radionuclide Transport Abstraction (CRWMS M&O 2000b)

Abstraction of Drift-Scale Coupled Processes (CRWMS M&O 2000c)

Abstraction of NFE Drift Thermodynamic Environment and Percolation Flux (CRWMS M&O 2000o)

6.4.1 Heating in the Drift Begins.

Abstraction of Drift-Scale Coupled Processes (CRWMS M&O 2000c)

Abstraction of NFE Drift Thermodynamic Environment and Percolation Flux (CRWMS M&O 2000o)

6.4.2 Heating Decreases, and Groundwater with Altered Composition Approaches and Enters Drifts (LOCATION 1 in Figure 2)

After the host rock temperature at the surface of the drift drops below boiling, groundwater begins to enter the drifts and backfill from the host rock driven by gravity (seepage) and capillary forces in the backfill. Several host rock properties and processes may influence the composition of groundwater approaching the drift. They are host rock temperature, host rock mineral identity and content, evaporation, precipitation, condensation of water vapor in the host rock, and constituents of the gas phase in the host rock. Reactions of cement grout and metallic components with groundwater and gases may also alter the composition of the approaching groundwater. After groundwater enters, reactions with in-drift gases may alter its composition at any location in the drift. Gas phase composition may be influenced by corrosion and other interactions among in-drift materials (e.g., cement grout, and metals).

Abstraction of Drift-Scale Coupled Processes (CRWMS M&O 2000c)

Abstraction of NFE Drift Thermodynamic Environment and Percolation Flux (CRWMS M&O 2000o)

EBS Radionuclide Transport Abstraction (CRWMS M&O 2000b)

Seepage/Cement Interactions (CRWMS M&O 2000h)

In-Drift Corrosion Products (CRWMS M&O 1999c)

In-Drift Gas Flux & Composition (CRWMS M&O 2000f)

In-Drifts Precipitates/ Salts Analysis (CRWMS M&O 2000j)

6.4.3 Groundwater Moves through the Backfill toward Other Engineered Components (LOCATION 1 in Figure 2)

Groundwater begins to move through the backfill toward other EBS components. Drip shields divert groundwater from contact with waste packages inside unless mechanical displacements or corrosion produce gaps in them.

EBS Radionuclide Transport Abstraction (CRWMS M&O 2000b)

6.4.4 Salts Precipitate in the Backfill and on the Drip Shield as the Groundwater there Evaporates (LOCATIONS 1 & 2 in Figure 2)

As a portion of the groundwater in the drift evaporates, salts precipitate in the backfill and on the drip shield and groundwater brines may result. Later, after some cooling occurs, groundwater brines form by redissolution of those salts. Knowledge of groundwater compositions on the drip shield is required to predict drip shield corrosion.

In-Drifts Precipitates/ Salts Analysis (CRWMS M&O 2000j)

6.4.5 Gaps May Form in Drip Shields Allowing Groundwater to Contact the Waste Packages (LOCATION 2 in Figure 2)

Gaps may form in the drip shields due to mechanical displacements of the invert or corrosion. Some groundwater may pass through those gaps, contacting the waste packages by dripping or by capillary movement in sand backfill that may have also passed through the gaps. Some or all of the groundwater that reaches the waste packages evaporates, and salts precipitate on the waste packages, possibly leaving brine by condensation or if the rate of water inflow exceeds the evaporation rate. The waste packages may also divert some of the groundwater directly to the invert.

EBS Radionuclide Transport Abstraction (CRWMS M&O 2000b)

In-Drifts Precipitates/ Salts Analysis (CRWMS M&O 2000j)

6.4.6 After Drift Temperatures Decrease, Reactions of Water Vapor with Deliquescent Salts Produce Brines (LOCATIONS 1 & 2 & 3 & 5 in Figure 2)

As in-drift temperatures decrease and relative humidity increases, water vapor may condense around and hydrate previously precipitated deliquescent salts in the backfill, on the drip shields, on the waste packages, and possibly in the invert. The result is formation of brines at those locations. Water vapor also condenses on deliquescent dust that may be present on waste packages, creating brine films.

In-Drifts Precipitates/ Salts Analysis (CRWMS M&O 2000j)

6.4.7 Reflux of Water May Occur inside the Drip Shields (LOCATION 3 in Figure 2)

It is conservative to include the possibility that water vapor may evaporate from the invert and condense inside drip shield. However, there are calculated results showing that, under the conditions used, the relative humidity underneath the drip shield did not reach the value of 100 percent required for condensation (CRWMS M&O 2000p, Section 6.5). It may be shown that condensation leading to reflux can be discounted. If reflux does occur, the condensate may flow onto the waste package and back into the invert. Thus, some brine may be created where salts have precipitated on the waste package, and brine compositions in the invert may be changed by the refluxing water.

6.4.8 Drip Shields and Waste Packages Corrode (LOCATIONS 2 & 3 in Figure 2)

The major corrosive processes are stress corrosion cracking in the welded lids of the waste package and general corrosion for both the drip shield and waste package. The composition of brine in contact with the waste package may be altered by reaction with metals (corrosion).

EBS Radionuclide Transport Abstraction (CRWMS M&O 2000b)

In-Drift Corrosion Products (CRWMS M&O 1999c)

6.4.9 Microbiological Activity Affects Corrosion Rates and Drift Gas Compositions (LOCATIONS 3 & 4 in Figure 2)

Bacteria may multiply in brine, where they can cause microbially induced corrosion (MIC) of the waste package and serve as a source term for microbial colloids in the in-drift colloid modeling. Microbiological activity may also alter in-drift gas compositions.

In-Drift Microbial Communities (CRWMS M&O 2000e)

6.4.10 Water Vapor Condensation and Seepage of Groundwater into Drifts Dilute Brines (ALL LOCATIONS)

Continued water vapor condensation on precipitated salts (deliquescence) results in formation of more dilute brines in the backfill, on drip shields, and on waste packages. Continued seepage into drifts also dilutes the brines. The following AMRs report analyses and models, quantitative and conceptual, of features and processes described above:

EBS Radionuclide Transport Abstraction (CRWMS M&O 2000b)

In-Drifts Precipitates/ Salts Analysis (CRWMS M&O 2000j)

6.4.11 Corrosion Penetrates Waste Packages, and Brines and Groundwaters Contact Waste Forms (LOCATIONS 3 & 4 in Figure 2)

Stress corrosion cracks and general corrosion penetrate the packages, allowing brine and groundwater to enter and contact waste forms. Compositions of water in contact with the waste forms may be determined by reactions with backfill, with previously precipitated salts formed by evaporation, with waste package metals altered by corrosion, and potentially with changing in-drift gas composition. The in-drift gas composition may be altered by corrosion reactions (e.g., oxygen, hydrogen). Some of the groundwater that has passed through gaps in the drip shield bypasses (or is diverted by) the waste package and may eventually reach the invert; some passes through corrosion gaps in the waste package and contacts the waste form.

EBS Radionuclide Transport Abstraction (CRWMS M&O 2000b)

Seepage/Backfill Interactions (CRWMS M&O 2000m)

In-Drifts Precipitates/ Salts Analysis (CRWMS M&O 2000j)

In-Drift Corrosion Products (CRWMS M&O 1999c)

In-Drift Gas Flux & Composition (CRWMS M&O 2000f)

6.4.12 Dissolved and Colloidal Materials Enter the Invert from Waste Forms by Groundwater Advection, and Potentially by Diffusion If Advection Does Not Dominate Transport (LOCATIONS 4 & 5 in Figure 2)

Composition of liquid water leaving the waste form through breaches in the waste package is influenced by waste form degradation and radionuclide mobilization.

In cases of significant transport by diffusion (advective transport does not dominate), molecular diffusion is expected to be faster than diffusion of colloidal particles, and diffusion of colloids may be shown to be insignificant to performance.

EBS Radionuclide Transport Abstraction (CRWMS M&O 2000b)

Develop the In-Package Chemistry Abstraction for TSPA-LA (CRWMS M&O 2000d)

In-Drift Colloids and Concentrations (CRWMS M&O 2000n)

6.4.13 Water in the Invert May Mix, and Dissolved and Colloidal Materials Enter the Unsaturated Zone by Groundwater Advection (and potentially Diffusion if advection does not dominate transport) (LOCATION 5 in Figure 2)

Water enters the invert along the following paths (CRWMS M&O 2000b):

A. Through the backfill and diverted by the drip shield

B. Through the drip shield and diverted along the outside of the waste package

C. Directly from inside the waste package after contact with the waste form.

Water streams entering the invert may mix, and they may interact with the invert materials. Water leaving the invert enters the host rock

In-Drifts Precipitates/ Salts Analysis (CRWMS M&O 2000j)

Develop the In-Package Chemistry Abstraction for TSPA-LA (CRWMS M&O 2000d)

EBS Radionuclide Transport Abstraction (CRWMS M&O 2000b)

Seepage/Invert Interactions (CRWMS M&O 2000i)

6.5 USE OF MODELS AND PARAMETERS IN TSPA

6.5.1 Identities and Uses of Parameters Transmitted to TSPA-SR by Sub-Model AMRs

Note that the physical and chemical environment parameters ultimately used in the TSPA largely depends on the actual input requirements of the dripshield and waste package corrosion models and the EBS transport model that are implemented in the TSPA. Parameters may be used by these TSPA abstraction models to calculate the following performance-related information:

(a) corrosion of drip shields and waste packages;

(b) salt precipitation, salt redissolution, and resulting groundwater compositions at one or more locations in the drifts and in released groundwater; and

(c) mobilization and release of materials from the engineered barrier system

(i) dissolved

(ii) colloidal

Specifically, the parameters named in Table 3 may be used in the TSPA calculations.

Table 1. Parameters available for TSPA in input EBS P/CE AMRs (compiled from *Develop the In-Package Chemistry Abstraction for TSPA-LA* (CRWMS M&O 2000d), *In-Drifts Precipitates/Salts Analysis* (CRWMS M&O 2000j), and *In-Drift Microbial Communities* (CRWMS M&O 2000e))

Applicable Process	Input Parameters to TSPA-SR
Drip Shield Corrosion	Groundwater composition: pH Chloride concentration Model to calculate mass of microbes per unit drift length
Waste Package Corrosion	Groundwater composition: pH Chloride concentration Model to calculate mass of microbes per unit drift length
EBS Transport by Colloids in Invert	Groundwater composition: Ionic strength Concentration of colloids
Radionuclide Mobilization and Release from Engineered Barrier System and Corresponding Groundwater Chemical Environment	Groundwater composition: pH Eh Ionic strength Total dissolved carbonate Chloride concentration Fluoride concentration Oxygen fugacity Carbon dioxide fugacity Concentration of colloids

6.5.2 Use of Abstracted Parameters and Information in TSPA Calculations

TSPA may use P/CE abstracted parameters and models to specify groundwater compositions and microbial masses for potential application at the following three locations

- Outer surface of the drip shield, treated in Section 6.5.2.1
- Outer surface of the waste package, treated in Section 6.5.2.2
- In the invert, treated in Section 6.5.2.3

See Figure 2 for a schematic diagram of the locations.

6.5.2.1 Specify Groundwater Composition on the Outer Surface of the Drip Shield

The groundwater composition parameters are pH, chloride concentration, and ionic strength given in *In-Drifts Precipitates/ Salts Analysis* (CRWMS M&O 2000j) as functions of temperature, relative humidity, the ratio of water evaporation flux to incoming groundwater seepage flux (called the relative evaporation flux, R^{es}), and carbon dioxide fugacity. The microbial mass may be calculated with a software code named MING V1.0 (CSCS 300018V1.0) that is given in *In-Drift Microbial Communities*, Section 6.4 (CRWMS M&O 2000e).

Parameter values in *In-Drifts Precipitates/ Salts Analysis* (CRWMS M&O 2000j) are based on an average J-13 well water composition which was used to reasonably approximate the incoming groundwater flux. For some time periods, incoming groundwater may have compositions different from J-13 well water. Also, chemical reactions in the drift, such as reactions of groundwater with cementitious grout, may alter groundwater composition outside the range covered. If necessary, additional precipitates/salts analyses should be done to extend the ranges of in-drift variables covered.

6.5.2.2 Specify Groundwater Composition on the Outer Surface of the Waste Package and Microbial Mass to Determine Waste Package Corrosion

The parameter sources, comments, and approximations for the groundwater composition on the outer surface of the drip shield also apply to the outer surface of the waste package.

6.5.2.3 Set Groundwater Composition in the Invert

Invert groundwater composition may affect the quantities of dissolved species and colloidal particles that enter the unsaturated zone. The stable colloid concentration may be determined as a function of ionic strength as described in *In-Drift Colloids and Concentrations* (CRWMS M&O 2000n). Quantities of dissolved species and colloidal particles may be useful to quantify radionuclides entering the unsaturated zone, a source term for calculating repository performance.

The relative quantities and flow paths of groundwater streams approaching the invert, chemical reactions, and evaporation of water can combine to determine the groundwater composition in the invert. Groundwater streams approaching the invert come from three sources: (a) from diversion by the drip shield, (b) from diversion by the waste package, and (c) from inside the waste package after it is breached, as given in *EBS Radionuclide Transport Abstraction* (CRWMS M&O 2000b). Those streams may mix. Diverted groundwater compositions can be determined as described in *In-Drifts Precipitates/Salts Analysis* (CRWMS M&O 2000j). Major water constituent dissolved concentrations from inside the waste package may be determined from *Develop the In-Package Chemistry Abstraction for TSPA-LA* (CRWMS M&O 2000d).

6.5.2.4 Calculate Groundwater Composition Released from Engineered Barrier System and Corresponding Groundwater Chemical Environment

Use the results from *Develop the In-Package Chemistry Abstraction for TSPA-LA* (CRWMS M&O 2000d) and information from a variety of external sources to calculate the composition and colloid content of groundwater leaving the invert. In-package chemistry parameters provided in *Develop the In-Package Chemistry Abstraction for TSPA-LA* (CRWMS M&O 2000d) are the following:

- pH
- Eh
- Ionic strength
- Total dissolved carbonate
- Chloride concentration
- Fluoride concentration
- Oxygen fugacity
- Carbon dioxide fugacity
- Concentration of Colloids

7. CONCLUSIONS

7.1 CONCEPTUAL MODEL SUMMARY

Knowledge of the physical and chemical environments in the drifts where waste is emplaced is available to quantify EBS processes and predict the composition of groundwater leaving the drift and entering the host rock. Among those environments are the temporal (a) evolution of groundwater flow paths in the drift and to the unsaturated zone of the host rock, and (b) composition of groundwater moving along those paths. Physical environment characteristics are needed to quantify groundwater movements in the drift that transport materials into the unsaturated zone. Brine composition values are needed to predict breaching of metallic engineered barriers by corrosion and to quantify processes that release and transport material from the waste forms to the host rock.

Seepage passes (by dripping) through the air gap above the backfill and then through the backfill. Capillary fluxes of groundwater also pass through the backfill. Reactions with ambient gases, evaporation, salt precipitation, and salt redissolution to form groundwater brines occur there. At the surface of the drip shield, groundwater is diverted and evaporation of groundwater, salt precipitation, and brine formation occur. The drip shield diverts groundwater fluxes until breached by mechanically induced gaps or corrosion. Groundwater then passes through breaches in the drip shield and contacts the surface of the waste package, where it is diverted to the invert until the waste package is breached by corrosion. That portion of groundwater that passes through breaches in the waste package, also contacts the waste forms. Reactions of groundwater with the waste forms mobilize radionuclides and change groundwater composition. Groundwater flow and molecular diffusion carry radionuclide-containing species from the waste forms inside the waste package to the invert.

Three streams of groundwater may enter the invert. They come from diversion by the drip shield, diversion by the waste package, and directly from the waste form (after breach of the drip shield and waste package). The groundwater streams diverted by the drip shield and waste package and coming directly from the waste form may mix in the invert. Reactions with ambient gases, evaporation, salt precipitation, and salt redissolution to form groundwater brines may also occur in the invert. Groundwater compositions in the invert resulting from evaporation, mixing and chemical reactions determine radionuclide solubility and stable colloid concentrations.

Invert groundwater carries dissolved and colloidal radionuclides across the invert/host rock interface into the unsaturated zone of the host rock. Transport to the unsaturated zone may also occur by molecular diffusion of dissolved constituents through the invert when advection does not dominate transport. Diffusion of colloidal particles is expected to be slower and may be shown to be insignificant to performance.

More detailed descriptions of these coupled processes are given in Section 6.4.

Parameters and models abstracted from resource AMRs, described in Section 6. and other input information may be used in the TSPA-SR to calculate the following performance-related information:

(a) corrosion of drip shields and waste packages;

(b) salt precipitation, salt redissolution, and resulting groundwater compositions at one or more locations in the drifts and in released groundwater;

(c) mobilization and release of materials from engineered barrier system

(i) dissolved

(ii) colloidal

Specifically, TSPA may use P/CE abstracted parameters and models as described in Section 6.4 to calculate groundwater compositions and microbial masses for potential application at the following three locations:

Outer surface of the drip shield, treated in Section 6.5.2.1

Outer surface of the waste package, treated in Section 6.5.2.2

In the invert, treated in Section 6.5.2.3

7.2 EVALUATION OF NRC ISSUE RESOLUTION STATUS REPORT CRITERIA

Regarding Section 4.2.1.1 (Data and Model Justification Acceptance Criteria), only criteria 1 and 2 were considered in this model, because the model is qualitative, not quantitative.

Regarding Section 4.2.1.2 (Data Uncertainty and Verification Acceptance Criteria), none of the criteria apply, because no data have been used in this model.

Regarding Section 4.2.1.3 (Model Uncertainty Acceptance Criteria), only criterion 1 was considered, because the model is qualitative only; no data or mathematical models were used. The model accounts for thermal-hydrologic properties through its use of the abstraction for seepage into the drift and the abstraction of the thermal-hydrologic response of the near-field environment with the NUFT code. Chemical effects are represented in the source term model through the effects of pH, Eh, and ionic strength on waste form dissolution rates and radionuclide solubility limits.

Regarding Section 4.2.1.4 (Model Verification Acceptance Criteria), none of the criteria apply, because the model is conceptual only; it includes no mathematical, or numerical models.

7.3 TECHNICAL PRODUCT RESOURCE INFORMATION IMPACT

This document may be affected by technical product resource information that requires confirmation. Any changes to the document that may occur as a result of completing the confirmation activities will be reflected in subsequent revisions. The status of the input information quality may be confirmed by review of the Document Input Reference System database.

7.4 FEP'S EVALUATION

Resource AMRs listed in Section 6. address FEPs that have not been screened out. This AMR does not directly address those FEPs.

7.5 LIMITATIONS

Use of this model is limited to providing an explanatory basis for the in-drift physical and chemical analyses performed by PAO.

8. INPUTS AND REFERENCES

8.1 DOCUMENTS CITED

Civilian Radioactive Waste Management System Management and Operating Contractor (CRWMS M&O) 1998. "Near-Field Geochemical Environment." Chapter 4 of *Total System Performance Assessment-Viability Assessment (TSPA-VA) Analyses Technical Basis Document.* B00000000-01717-4301-00004 REV 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19981008.0004.

CRWMS M&O 1999a. *Physical and Chemical Environment Abstraction Model for TSPA-LA.* TDP-WIS-MD-000007 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990902.0449.

CRWMS M&O 1999b. *Conduct of Performance Assessment.* Activity Evaluation, September 30, 1999. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19991028.0092.

CRWMS M&O 1999c. *In Drift Corrosion Products.* ANL-EBS-MD-000041 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20000106.0438.

CRWMS M&O 2000a. *Engineered Barrier System Degradation Modes & Features, Events, and Processes Abstraction.* ANL-WIS-PA-000002 REV 00. Las Vegas, Nevada: CRWMS M&O. Submit to RPC URN-0199

CRWMS M&O 2000b. *EBS Radionuclide Transport Abstraction.* ANL-WIS-PA-000001 REV 00. Las Vegas, Nevada: CRWMS M&O. Submit to RPC URN-0208

CRWMS M&O 2000c. *Abstraction of Drift Scale Coupled Processes.* ANL-NBS-HS-000029 REV 00. Las Vegas, Nevada: CRWMS M&O. Submit to RPC URN-0032

CRWMS M&O 2000d. *In-Package Chemistry Abstraction for TSPA-LA.* Input Transmittal 00163.T. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20000327.0214.

CRWMS M&O 2000e. *In Drift Microbial Communities.* ANL-EBS-MD-000038 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20000331.0661.

CRWMS M&O 2000f. *In-Drift Gas Flux & Composition.* ANL-EBS-MD-000040 REV 00. Las Vegas, Nevada: CRWMS M&O. Submit to RPC URN-0195

CRWMS M&O 2000g. *Miscellaneous Waste Form FEPs.* Input Transmittal 00149.T. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20000317.0471.

CRWMS M&O 2000h. *Seepage/Cement Interactions.* ANL-EBS-MD-000043 REV 00. Las Vegas, Nevada: CRWMS M&O. Submit to RPC URN-0123

CRWMS M&O 2000i. *Seepage/Invert Interactions.* ANL-EBS-MD-000044 REV 00. Las Vegas, Nevada: CRWMS M&O. Submit to RPC URN-0197

CRWMS M&O 2000j. *In-Drift Precipitates/Salts Analysis.* ANL-EBS-MD-000045 REV 00. Las Vegas, Nevada: CRWMS M&O. Submit to RPC URN-0198

CRWMS M&O 2000k. *FEPs Screening of Processes and Issues in Drip Shield and Waste Package Degradation.* Input Transmittal 00150.T. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20000317.0480.

CRWMS M&O 2000l. *Waste Form Colloid-Associated Concentrations Limits: Abstraction and Summary.* Input Transmittal 00175.T. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20000328.0644.

CRWMS M&O 2000m. *Seepage/Backfill Interactions.* ANL-EBS-MD-000039 REV 00. Las Vegas, Nevada: CRWMS M&O. Submit to RPC URN-0194

CRWMS M&O 2000n. *In-Drift Colloids and Concentrations.* ANL-EBS-MD-000042 REV 00. Las Vegas, Nevada: CRWMS M&O. Submit to RPC URN-0196

CRWMS M&O 2000o. *Abstraction of Near Field Environment Drift Thermodynamic Environment and Percolation Flux.* ANL-EBS-HS-000003 REV 00. Las Vegas, Nevada: CRWMS M&O. Submit to RPC URN-0039

CRWMS M&O 2000p. *In-Drift Thermal-Hydrological-Chemical Model.* ANL-EBS-MD-000026 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20000113.0488.

8.2 CODES, STANDARDS, REGULATIONS, AND PROCEDURES

AP-3.10Q, Rev. 2, ICN 0. *Analyses and Models.* Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20000217.0246.

DOE (U.S. Department of Energy) 2000. *Quality Assurance Requirements and Description.* DOE/RW-0333P, Rev. 9. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.19991028.0012.

NRC (U.S. Nuclear Regulatory Commission) 1999. *Issue Resolution Status Report Key Technical Issue: Evolution of the Near-Field Environment.* Rev. 2. Washington, D.C.: U.S. Nuclear Regulatory Commission. ACC: MOL.19990810.0640.

NLP-2-0, Rev. 5. *Determination of Importance Evaluations*, Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19981116.0120.

QAP-2-0, Rev. 5. *Conduct of Activities.* Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980826.0209.

QAP-2-3, Rev. 10. *Classification of Permanent Items*, Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990316.0006.

9. ATTACHMENTS

Attachment	Title
I	List of Acronyms

ATTACHMENT I
LIST OF ACRONYMS AND ABBREVIATIONS

ACC	Accession Number
AMR	Analysis/Model Report
CRWMS M&O	Civilian Radioactive Waste Management System Management and Operating Contractor
DOE	United States Department of Energy
EBS	Engineered Barrier System
FEP	Features, Events, and Processes
IRSR	Issue Resolution Status Report
M&O	Civilian Radioactive Waste Management System Management and Operating Contractor
NFE	Near Field Environment
NRC	U.S. Nuclear Regulatory Commission
PAO	Performance Assessment Operations
P/CE	Physical and Chemical Environment
QA	Quality Assurance
R^{es}	Relative Evaporation Rate
SZ	Saturated Zone
TBV	To Be Verified
TH	Thermal-hydrologic
THC	Thermal-Hydrologic-Chemical
TSPA	Total-System Performance Assessment
TSPA-LA	Total-System Performance Assessment-License Application
TSPA-SR	Total-System Performance Assessment-Site Recommendation
TSPA-VA	Total-System Performance Assessment-Viability Assessment
UZ	Unsaturated Zone

WF	Waste Form
YMP	Yucca Mountain Site Characterization Project