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NM5507

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT

1. QA: QA

ANALYSIS/MODEL COVER SHEET

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: Determine potential for in-drift contents and processes to affect in-drift gasses.	Describe use:

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OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
ANALYSIS/MODEL REVISION RECORD

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1. PURPOSE

As directed by a written development plan (CRWMS M&O 1999a), changes in the in-drift gas flux and composition resulting from the thermal perturbation of the geosphere and reactions of the ambient gases with introduced materials of the engineered barrier system (EBS) are to be evaluated. The purpose of this analysis is to assist Performance Assessment Operations (PAO) and its Engineered Barrier Performance Department in modeling the geochemical environment within a repository drift, thus allowing PAO to provide a more detailed and complete in-drift geochemical model abstraction and to answer the key technical issues (KTI) raised in the Nuclear Regulatory Commission (NRC) Issue Resolution Status Report (IRSR) for the Evolution of the Near-Field Environment (NFE) Revision 2 (NRC 1999).

The scope of this document is to evaluate the need to consider possible changes to the in-drift gases, particularly carbon dioxide (CO_2), oxygen (O_2), nitrogen (N_2) and steam (H_2O) in future performance assessments (PA), based on the conceptual framework for in-drift gas flux and composition discussed in this report. The decision documented in this report will be used to determine whether chemical changes to in-drift gases must be included in future PA analyses.

This analysis focuses on changes that may affect CO_2 and O_2, and discusses N_2 and steam in less detail. A key parameter, gas flux into the drift, (to be documented in future revision to *Drift-Scale Coupled Processes(DST and THC Seepage) Models* (CRWMS M&O 2000a) and *Abstraction of Drift-Scale Coupled Processes* (CRWMS M&O 2000b) was not available at the time this document was prepared, so the previous model for in drift gas, documented in the TSPA-VA (CRWMS M&O 1998) provided the estimates of gas flux and composition boundary conditions. Gas flux into the drift has also been calculated as reported in *Physical and Chemical Environment Model* (CRWMS M&O 2000c). The results of the calculation reported in that document were in progress and so were not available for use in the analysis reported in this document, but will be considered in preparing later revisions. This analysis discusses the processes that are potentially important in affecting gas composition in the drift and uses mass balance considerations to evaluate the importance of potential sources and sinks for CO_2 and O_2. An analytical approach for tracking gas composition relative to incoming gas composition over time was not specifically developed because of the lack of an Incoming Gas Model that could be used to provide time-dependent boundary conditions.

2. QUALITY ASSURANCE

The Quality Assurance (QA) program applies to the development of this (conceptual model, model, or analysis - dependent on purpose/scope) documentation. The Performance Assessment Operations responsible manager has evaluated the technical document development activity in accordance with QAP-2-0, *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 to *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 SOFTWARE

No software requiring development and controls in accordance with AP-SI.1Q, *Software Management*, was used in the development of this document.

3.2 MODELS

A conceptual model of the various factors which may influence in-drift gas flux and composition is evaluated in this report. This simple conceptual model consists of the ambient gas flux through the rock mass as a boundary condition and the various mechanisms that may operate to alter repository gases. The conceptual model was developed for use in Chapter 4 of the Total System Performance Assessment-Viability Assessment (TSPA-VA) Technical Basis Document (CRWMS M&O 1998, DTN: MO9807MWDEQ3/6.001). That model is extended in this report to consider the major mechanisms that may operate under repository conditions to affect in-drift gas flux and composition. The conceptual model for gas flux into the drift as documented in CRWMS M&O (1998) for TSPA-VA is appropriate for use in this analysis. A brief summary of the TSPA-VA conceptual model is found in Section 6.1.

4. INPUTS

4.1 DATA AND PARAMETERS

The data and parameters used in this document were taken from other Analysis/Model Reports and other Yucca Mountain Program documents to provide compatibility among the various project modeling and analysis efforts. Specific inputs are discussed below.

Tables 1 and 2 below document the masses and compositions of the various metals and alloys included in the repository. These tables are created from results derived in the AMR *In Drift Microbial Communities* (CRWMS M&O 2000d) and are provided in the following DTNs: MO0001SPARSD38.014, MO0003SPAARD38.026, MO0003SPAARD38.023, MO0001SPAAWP38.010, MO0001SPAWPD38.009, MO0001SPACSS38.017, and MO0001SPANEU38.018.

The expansive cement (Portland Type k) used to grout the rock bolts in the non-lithophysal lithology of the host rock contains 45.4% Ca by weight, as calculated from the calcium content of the mineral composition (DTN: MO9909SPATYPEK.004) using the following relationship:

$$M_{Ca} = \Sigma \left([40.1 \text{x } N/GFW_{mineral}] \text{x } A_{mineral} \right) \qquad \text{(Eq. 1)}$$

summed over all mineral phases present in the grout.

Where: 40.1 = Atomic Weight of Ca
N = number of Ca atoms in mineral formula
GFW = gram formula weight of each mineral
A = abundance of each mineral phase in the grout (expressed as a fraction of total grout)

All atomic weight and gram formula weight data are accepted data from the CRC Handbook for Chemistry and Physics (Weast, 1979).

Some repository design information necessary for the mass balance calculations is contained in YMP Input Transmittal PA-SSR-99218.Ta (CRWMS M&O 1999c).

Estimated gas influx to the drifts over time is drawn from the TSPA-VA, Section 4.6.2.1 (CRWMS M&O 1998) and is drawn from a spreadsheet found in the following DTN: MO9807MWDEQ3/6.001.

Table 1. Total masses and percentages of metals/alloys in a meter segment of repository drift .

Material	Quantity (kg/m)[a]	Composition (%)						
		Fe	C	Mn	V	Cu	Source	QA Status[b]
Rockbolt Sets	48	99.02	0.79				MO0001SPARSD38.014	A
Welded Wire Fabric (WWF)	70	98.8	1.0				MO0003SPAARD38.026	U
Gantry Rail	134	97.59	0.82	1.0			MO0001SPARSD38.014	A
Rail Fittings	10.0	73.11	0.17	1.24	0.11	25.0	MO0003SPAARD38.026	U
Steel Sets	369	97.48	0.23	1.65	0.15		MO0001SPARSD38.014	A
Conductor Bar Ftg.s	0.2	97.48	0.23	1.65	0.15		MO0001SPARSD38.014	A
Communication Cable	0.79		42.82			50.0	MO0003SPAARD38.026	U
Steel Invert	587	97.48	0.23	1.65	0.15		MO0001SPARSD38.014	A
Total (kg/m)	1219	1187	4.73	17.2	1.45	2.90		U

Notes:
a – source: DTNMO0003SPAARD38.023 – Unqualified Data
b – U = Unqualified Data
A = Accepted Data

Table 2. Total masses and percentages of metals/alloys within a meter segment of a 21 PWR waste package based on the SR.

Material	Quantity (kg/m)[a]	Composition (%)								Source	QA Status
		Fe	C	Mn	Ni	Mo	Ti	Al	Cr		
ASTM B 575 (C-22)	1456 (summation of sources)	6.00	0.02		50.0	14.5			22.5	MO0001SPAWPD38.009	A
ASTM 316L	128	61.8	0.03	2.00	14.0	3.00			18.0	MO0001SPAWPD38.009	A
ASTM 316NG	2106	61.8	0.02	2.00	14.0	3.00			18.0	MO0001SPACSS38.017	A
Al Type 6061	63	0.70		0.15			0.15	96.0	0.35	MO0001SPAWPD38.009	A
Neutro - nit A 978	387	66.7	0.04		13.0				18.5	MO0001SPANEU38.018	U
ASTM A 516	1073	97.9	0.27	1.30						MO0001SPAWPD38.009	A
ASTM B 265 (Ti Grade 7)	563	0.30	0.10				99.1			MO0001SPAWPD38.009	A
Total (kg/m)	5776	2779	4.37	58.7	1091	278	558	60.5	778		

Notes:
a – Source: DTNMO0001SPAAWP38.010 – Unqualified Data
b – U = Unqualified Data
A = Accepted Data

4.2 CRITERIA

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 Evolution of the Near-field environment (NFE) key technical issue (KTI) 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 (FEP's) that apply to this report.

4.2.1 NRC IRSR Criteria

Evaluations of the criteria are discussed in Section 7.3. The following acceptance criteria are from section 4.3.1 of the NFE IRSR and are provided as representative examples of the criteria in the other cited sections. For specific acceptance criteria for each of the sections cited, the NFE IRSR should be used.

4.2.1.1 Data and Model Justification Acceptance Criteria

1. Consider data relevant to both temporal and spatial variations in conditions affecting coupled THC effects on the chemical environment for radionuclide release were considered. [NRC (1999), Sections 4.2.1, 4.3.1, and 4.4.1]

2. Coupled THC processes must properly 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 4.2.1, 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 4.2.1, 4.3.1, and 4.4.1]

4. A nutrient and energy inventory calculation should be used to determine the potential for microbial activity that could impact the waste package (WP) chemical environment. [NRC (1999), Sections 4.2.1, 4.3.1, and 4.4.1]

5. Should microbial activity be sufficient to allow microbial influenced corrosion (MIC) of the WP, then the time-history of temperature, humidity, and dripping should be used to constrain the probability for MIC. [NRC (1999), Sections 4.2.1, 4.3.1, and 4.4.1]

6. 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 4.2.1, 4.3.1, and 4.4.1]

7. 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, U.S. Department of Energy (DOE) has identified specific plans to acquire the necessary information as part of the performance confirmation program. [NRC (1999), Sections 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 are technically defensible and reasonably account for uncertainties. [NRC (1999), Sections 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 4.2.1, 4.3.1, and 4.4.1]

3. Evaluation of coupled THC processes must properly consider the uncertainties in 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 4.2.1, 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 must be consistent with available data. [NRC (1999), Sections 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 4.2.1, 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 WP, materials and groundwater, which, in turn, may affect the chemical environment for radionuclide release. [NRC (1999), Sections 4.2.1, 4.3.1, and 4.4.1]

2. Investigate alternative modeling approaches consistent with available data and current scientific understanding, and their results and limitations must be appropriately considered. [NRC (1999), Sections 4.2.1, 4.3.1, and 4.4.1]

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

2. 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 4.2.1, 4.3.1, and 4.4.1]

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

4.2.2 YMP Features, Events and Processes (FEP's)

Table 3 below gives a listing of Yucca Mountain Project FEP's (CRWMS M&O 1999d) that are or may be potentially discussed in this document. YMP FEP # and NEA Category are part of the database search properties and are provided for convenience.

Table 3. A listing of YMP FEP's that pertain to this document.

YMP FEP #	NEA Category	FEP Name
2.1.02.02.09	2.1.09z	Dissolution chemistry (in waste and engineered barrier system)
2.1.09.02.00	3.2.01i	Interaction with corrosion products
2.1.09.02.02	2.1.09bd	Effects of metal corrosion (in waste and engineered barrier system)
2.1.09.04.02	2.1.09r	Speciation (in waste and engineered barrier system)
2.1.09.04.09	3.2.02h	Solubility and precipitation (contaminant speciation and solubility)
2.2.08.03.18	3.2.03m	Groundwater chemistry (sorption/desorption processes)
2.1.06.02.00	2.1.06g	Effects of rock reinforcement materials
2.1.06.06.00	WP-1	Effects and degradation of drip shield
2.1.12.03.01	2.1.12ai	Chemical effects of corrosion
2.1.06.05.00	2.1.05p	Degradation of invert and pedestal
2.1.03.01.00	2.1.03a	Corrosion of waste containers
2.1.08.07.02	2.1.03ay	Properties of failed canister
2.1.09.02.04	2.2.08v	Chemical buffering (canister corrosion products)
2.1.12.03.01	2.1.12ai	Chemical effects of corrosion
2.1.09.05.00	2.1.09bm	In-drift sorption
2.1.09.05.02	3.2.03b	Sorption

Any resolution of these FEP's is discussed in Section 7.6 below.

4.3 CODES AND STANDARDS

4.3.1 Codes

This AMR was prepared to comply with the DOE interim guidance (Dyer 1999) which directs the use of the proposed NRC high-level waste rule, 10 CFR Part 63. Relevant requirements for performance assessment from Section 114 of that document are: "Any performance assessment used to demonstrate compliance with Sec. 113(b) shall: (a) Include data related to the geology, hydrology, and geochemistry ... used to define parameters and conceptual models used in the assessment. (b) Account for uncertainties and variabilities in parameter values and provide the technical basis for parameter ranges, probability distributions, or bounding values used in the performance assessment. ... (g) Provide the technical basis for models used in the performance assessment such as comparisons made with outputs of detailed process-level models ... ."

4.3.2 ASTM Standards

No ASTM standards apply to this document

5. ASSUMPTIONS

5.1 ASSUMPTION 1

All metals and alloys in the disposal drifts are considered equivalent to iron for the purpose of the mass balance calculation [used in Section 6.2.2.] This assumption is used only to simplify the calculation of the amount of oxygen consumed in corrosion of the metal. Other metals are present in the disposal drifts, particularly in the spent fuel wastes and associated packages and containers, but this assumption is expected to introduce an error of less than one order of magnitude in the calculated oxygen demand. This assumption is justified because the transition metals (Mo, Ni, Co, and Cr) are present in quantities less than the iron present, and their effect is to increase the corrosion resistance of the metal in which they are included. . These metals all require at least as much O_2 stoichiometrically for oxidation as iron. This degree of uncertainty will have no effect on the mass balance calculation contained in this document. This assumption bounds the amount of oxygen that can be used and does not require further confirmation.

5.2 ASSUMPTION 2

The carbon contained in the mild steel in the disposal drifts is assumed to not act as a significant source of CO_2 to the in-drift gas mixture [used in Section 6.2.1.] The calculation in section 6.2.1 below determined that more than ample CO_2 is available from the gas flux through the drifts to completely saturate available CO_2 sinks, and therefore CO_2 from mild steel need not be considered in this analysis. The amount of carbon in carbon steel in the drifts, based on the information in Table 1 in Section 4.1 is approximately 4.7 kg/m (392 moles C/m) of drift. This amount of carbon if oxidized would produce 392 moles/m of CO_2 over the time required to oxidize the mild steel and release the carbon. This amount of CO_2 is very small in comparison with the amount of CO_2 flux anticipated in the drifts as discussed in Assumption 3 (Section 5.3) below.

5.3 ASSUMPTION 3

The gas fluxes through the host rock calculated for the TSPA-VA (CRWMS M&O 1998) documented in a spreadsheet (DTN: MO9807MWDEQ3/6.001) were used as the basis for some of the calculations in Section 6.2. These calculated fluxes do not necessarily reflect current designs and so are considered to be verified (TBV). They will be replaced with new data from an abstraction of the in drift gas flux to be documented in a future revision to the *Abstraction of Drift Scale Coupled Processes* AMR (CRWMS M&O 2000b) in future revisions of this document. This assumption requires further confirmation.

5.4 ASSUMPTION 4

Gas composition throughout the drift is assumed to be homogeneous (used throughout). This is justified because gas transport rates are sufficiently high, even if only diffusive movement of gas constituents is considered, to mix gases in this unsaturated environment at the scale of a drift diameter. No further confirmation of this assumption is needed.

5.5 ASSUMPTION 5

The simplifying assumption is made that all of the waste packages can be represented by using the 21-PWR waste package material compositions and amounts (used throughout). This assumption is justified because the 21-PWR packages are the most common package identified for disposal, and the assumption only affects the mix of corrosion-resistant metals used for the oxygen mass balance calculation. The calculation is not sensitive to differences in the mix of corrosion-resistant metals. This assumption needs no further confirmation.

6. ANALYSIS/MODEL

This Analysis/Model Report (AMR) provides the basis for constraining the values of the gas flux and composition in the potential emplacement drifts in terms of the major geochemical constituents carbon dioxide (CO_2,) oxygen (O_2), nitrogen (N_2), and steam or water vapor (H_2O). This work (1) discusses the important processes affecting gas composition in the drift, and (2) uses mass balance considerations for the major potential sinks of both oxygen and carbon dioxide to assess whether these sinks may affect the gas composition within the drift relative to the composition and flux of these constituents entering the drift. The approach used here can be used to track changes in gas flux and composition when improved boundary conditions over time are available from the *Abstraction of Drift Scale Coupled Processes* (CRWMS M&O 2000b).

Major processes to be considered within this system include ambient and thermally perturbed fluxes of gas into the drift from the geosphere, fluxes of aqueous solutions into the drift, possible source terms for gas constituents in water just outside the drift, boiling of the water in the emplacement drift, and possible chemical reactions among the water-gas-introduced materials in the emplacement drift. Because the required parameters are not finalized, this work uses the time varying boundary conditions for the compositions and fluxes of gas and aqueous solutions that are supplied by external models as described in the TSPA-VA (CRWMS M&O 1998, DTN: MO9807MWDEQ3/6.001). Information on the inventory, masses, and compositions of the

introduced materials is provided by an input transmittal (CRWMS M&O 1999c) as listed in Section 4. The major introduced materials that may act as sources or sinks for the major constituents in the gas phase are evaluated for their potential to alter the in-drift gas composition from the externally supplied gas composition based on the flux of each constituent considered. If the boundary condition composition of any gas constituent entering the drift would be decreased by more than an order of magnitude, consideration of the compositionally-driven diffusion of that constituent from the water just outside the drift may be required for a more realistic analysis. Such additional potential sources would be added to that given by the supplied boundary conditions of gas flux and seepage flux. Specifically, mass balance calculations considering the major potential sinks of both oxygen and carbon dioxide are used to assess whether the sinks may affect the gas composition within the drift relative to the rate these constituents are supplied to the drift.

The conceptual model that is applied here (CRWMS M&O 1998, DTN: MO9807MWDEQ3/6.001), referred to as the In-Drift Gas sub-model of the In-Drift Geochemical Environment, provides context for using the above analyses. This sub-model can be stated as follows: if analyses of the major sink terms evaluated show substantial capacity to affect the incoming gas composition (by at least an order of magnitude), for meaningful performance assessment time scales (i.e., hundreds of years) then the composition of gas in the drift is adjusted from the boundary condition values in the appropriate manner. Otherwise, it is taken to be that imposed by the boundary conditions of the drift. In addition, this model assumes that the gas composition throughout the drift is homogeneous because gas transport rates are sufficiently high, even if only diffusive movement of gas constituents is considered, to mix gases in this unsaturated environment at the scale of a drift diameter (see Assumption 4 in Section 5.4). For consideration of locally-developed gas heterogeneity, more detailed process models of the hydrology for the In-Drift environment would be needed.

6.1 BACKGROUND INFORMATION

The amounts of various components of the in-drift gas are affected by a number of different process and conditions. These are divided into *sources* and *sinks* of each component. The efficiency of each source or sink may vary as a function of repository conditions, which may be approximated by different time stages or spatial zones of roughly similar conditions. Each potential source or sink will be discussed separately, including conceptual analysis of the behavior, controls and time-dependence of each.

6.1.1 In-Drift Gas Sources

Gases in the drift can arise from several sources or through several processes. These include infiltration through the rock from the land surface, exsolution from groundwater, bacterial action, gas production from corrosion, radiolysis, and decay of radionuclides. The efficiency of each of these processes varies as a function of repository conditions, and therefore varies with time as the repository goes through heating and cooling over the first several thousand years after closure. The gases expected to be of importance in system performance are the major gas constituents: steam (H_2O), oxygen (O_2), nitrogen (N_2) and carbon dioxide (CO_2). Although nitrogen is not expected to have a significant impact on chemical conditions in the drifts, it is included because

of its potential importance to microbial communities. The TSPA-VA (CRWMS M&O 1998, Section 4.4) discusses the sources of these gases and the mountain-scale processes affecting their quantities. The following discussion of processes controlling gas flux and composition is taken from the TSPA-VA (CRWMS M&O 1998, Section 4.2.3.1.1)[Note: references in all the quoted text below are from the cited source documents and are not included in Section 8 (References) of this report.]:

> "Because gas is less soluble at higher temperature, heating drives dissolved gases out of the water and into the gas phase. Rapid gas movement in the fractures may transport those dissolved gas constituents away from the heated water they came from and toward cooler water (that is, down the temperature gradient) where they can redissolve. This process tends to deplete the heated water and enrich the cooler water in these gas species. As the temperature of the mountain increases farther away from the repository, these gas species are remobilized and transported farther away from the drifts in a continual process of revaporization and redissolution. In the rock near the heat sources, temperatures will rise above the boiling point of water, generating abundant steam, causing an overall dilution of the air component.
>
> The major source of both oxygen and nitrogen is the atmosphere, so dilution of these two constituents by steam (from boiling) is accounted for by a direct reduction in their atmospheric partial pressures. For carbon dioxide, the system is somewhat more complex. Measurements of gas compositions from various UZ boreholes demonstrate that UZ CO_2 gas concentrations are elevated above atmospheric CO_2 partial pressures (about 350 ppmv—parts-per-million by volume) by about a factor of three (CRWMS M&O 1998a, Section 6.2.7.2, pp. 6.2-40). The values of UZ pore-gas composition analyzed for the site indicate that the CO_2 content of pore gases tends to average about 1000 ppmv (CRWMS M&O 1998a, Section 5.3.4.2.4.6, pp. 5.3-173). These elevated values could be the result of mixing of CO_2-rich gases generated in the soil zone with the rest of the gas volume of the mountain (CRWMS M&O 1998a, Section 5.3.4.2.4.6, p. 5.3-173).
>
> Because the rock contains the mineral calcite ($CaCO_3$) and there is a nonnegligible amount of dissolved carbonate in the water, these phases may act as sources of carbon dioxide that must be accounted for in the assessment of the air composition diluted by steam (Hardin et al. 1998, Sections 5.7.1 and 6.2.1). However, because gas flow is much more rapid than water flow, the NFGE model assumes that the water composition will be primarily controlled by the gas composition diluted by steam for most of the thermal period. Nevertheless, there are indications from water compositions in the single-heater test that carbon dioxide could be released to the gas phase during the heating stage (Hardin et al. 1998, Sections 5.7.1, 6.2.1 and 6.6). Therefore, a brief period with an elevated level of carbon dioxide in the air, which is then diluted by steam, was included at the start of the model to represent these potential sources of carbon dioxide.
>
> The incoming-gas model also assesses constraints on the fluxes of the gas constituents into the drift. These values are used in analyses that evaluate the potential for depletion of these constituents by reaction with the solids in the drift, and the potential effects on water–solids chemistry of those reactions and the potential microbial growth (discussed below). For each of the gas constituents in the model, the cumulative gaseous flux of that chemical component into the drift is given by the product of the cumulative gas phase flux and the fraction of that constituent in the gas for a given period. In the conceptual models for the gas and water/solids chemistry in the drift, the fluxes of these gas constituents that could be derived from their dissolved counterparts in the water flux were also included. For this model, the fluxes of the dissolved gas constituents were based on the percolation flux for the drift cross-section. This water flux is larger than that given by the seepage model, which only has a fraction of the percolation flux entering the drift. Because gaseous diffusion for carbon dioxide or oxygen gas species is relatively rapid at this scale, the gas composition may be buffered by water just outside the drift. Therefore, this larger water flux should represent a more realistic bound on the masses of these gas constituents available for reaction in the drift (see Section 4.4)."

Each potential additional source of in-drift gas is discussed below.

6.1.1.1 Radiolysis

Radiolysis is chemical decomposition by the action of radiation. For example, the breakdown of water at the waste package by radiation will produce hydrogen (H_2) and oxygen (O_2), which will contribute to the in-drift gas inventory. The amount of gas produced depends on 1) the availability of water, and 2) the production of radiation of sufficient energy to break the H-O bond in water. The first requirement, water availability, will be strongly affected by repository conditions, particularly the temperature of the waste packages. It is anticipated that the temperature at and near the surface of the waste packages will be higher than 100°C for several hundred years after repository closure (DOE 1998, Section 3.2.3). The availability of water at or near the waste packages will be very limited during the thermal period, when water vapor only is expected in the vicinity of the waste. The production of suitable radiation depends on the initial radionuclide inventory and time-dependent decay and daughter in-growth profiles of the various types of waste, and thus will decrease rapidly during the thermal period (DOE 1998, Section 3.5.1.5). As a result of these factors, radiolysis is not expected to contribute significant amounts of gas to the in-drift environment.

6.1.1.2 Gases in the Waste Packages

Several gases are produced as a direct result of decay of radioactive elements and are released to the drifts when the waste form degrades (Walker and Miller 1984). For example, radon (Rn) is an inert radioactive gas with isotopes of relatively short half-lives (less than 4 days). Any radioactive gases with a short half-life relative to the lifetime of the repository gas dynamics will not affect the drift gas balance. Helium (He) is a stable inert gas formed as a result of alpha (helium nucleus) decay of many radionuclides. Since helium is an inert gas, its presence will not affect in-drift chemical conditions. The only possible effect of increased amounts of inert gases would be to displace other gases in the repository, thus decreasing the partial pressures of gases of chemical importance, O_2 and CO_2. The total amount of ^{14}C contained in the wastes is a few thousand curies (DOE 1998, Section 3.5.1) at repository closure. Each curie of ^{14}C contains 0.224g of carbon (calculated using Equation 4.7 of Faure, 1986). Oxidation of the ^{14}C contained in the wastes will result in production of approximately 16 moles (360 liters at 22.4 moles/liter at standard temperature and pressure) of CO_2 per 1000 curies of ^{14}C, for a total CO_2 production of a few thousand liters, which will not all be released at the same time. In addition, the ^{14}C will continually decay with a half-life of approximately 5,730 years. Gases from the waste form are not anticipated to be releases from the waste packages until after the packages are breached, expected to be at least tens of thousands of years after repository closure (DOE 1998, Section 3.4.3). The contribution of these waste package gases to the composition of in-drift gases is negligible. Including them in the calculation would result in a small decrease in the partial pressure of atmospheric gases within the drifts, but would not change any of the chemical or geochemical processes that will affect atmospheric gases. The In-Drift Gas model does not address the potential contribution of any radionuclides, including gases, to radionuclide migration or dose.

6.1.1.3 Microbial Activity

The activity of microorganisms can generate gases as a result of metabolic activity, as discussed in the TSPA-VA (CRWMS M&O, 1998, Section 4.6.2.3.3.4). The conceptual model of microbial

activity is presented in detail in *In-Drift Microbial Communities* (CRWMS M&O 2000d), but the aspect of that model most significant to in-drift gas flux and composition is that the microorganisms will consume O_2, N_2 and CO_2 and produce CO_2. The TSPA-VA found that the amount of CO_2 produced or O_2 consumed as a result of microbial activity would not have a significant effect on bulk chemistry in the drifts because of the small amount of biomass expected to be present at any time. The model discussed in that document has recently been refined (CRWMS M&O, 2000d), but the conclusion reported in the earlier document (CRWMS M&O, 1998) has not changed as a result of the recent work.

6.1.2 In-Drift Gas Sinks

Gases in the drift can be consumed by several mechanisms. These include solution into groundwater, reaction with rock and repository engineered materials, displacement by other gases and vapors, and bacterial action. The rate of each of these processes varies as a function of repository conditions, and therefore varies with time and location within the drifts as the repository goes through heating and cooling over the first several thousand years after closure.

6.1.2.1 Groundwater Solution

As higher concentrations (partial pressures) of various gases accumulate as the result of the processes discussed in the previous section, some of those gases may dissolve in local groundwater, especially if that groundwater is percolating downward from the surface or from some other source where dissolved species are not saturated. This process is likely to be important during the thermal period, when downward-moving groundwater is likely to be cooler than materials in and near the disposal drifts. This more highly charged groundwater continues to percolate downward into still cooler regions, so this mechanism will result in removal of a significant amount of CO_2, which increases its solubility in water as temperature decreases from the drifts and vicinity.

6.1.2.2 Reaction with Rock and Repository Materials

This category of processes will likely have the greatest impact on repository gas composition, at least during the first 10,000 years after closure. The processes in this category include gas-rock interactions, carbonation of the calcium contained in cementitious materials such as grout in the rock support system, corrosion of carbon steels in the drifts, corrosion of stainless steels and other alloys and metals associated with the waste packages, and corrosion/dissolution of spent fuel. All of these mechanisms are chemical reactions, which proceed at rates controlled by chemical conditions and temperature, among other factors. The cement used for grouting the rockbolts in the drifts requiring support contains calcium, which will consume CO_2 during carbonation reactions (CRWMS 2000e). Alteration of steels and alloys will produce metal-oxide and -hydroxide corrosion products within the drift and may form metal-silicate minerals (CRWMS M&O 1999e). As the iron (Fe) and other metals in the steel and alloys oxidize, they represent a sink for oxygen and could be a mechanism for generating locally reducing conditions if the oxygen flux into the potential drift is sufficiently low (CRWMS M&O 1999e, Section 6), as may occur during the thermal period. The quantities and compositions of the metals used in the evaluated design are given in Tables 1 and 2 in Section 4.1.

6.1.2.3 Displacement

Production of water vapor will have the effect of displacing gas from the disposal drifts. This mechanism is likely to be very significant during the thermal period, when water in and near the disposal drifts is converted to steam by either boiling or enhanced evaporation (if the in-drift temperatures do not exceed the boiling point), as discussed in Section 6.1.1.1, above. This effect will decrease as the temperature drops, and ambient conditions, including gas flux, are reestablished. Radiolytic gas production and the contribution of gases in the waste are expected to be of minor importance with respect to displacement, as discussed in Sections 6.1.1.1 and 6.1.1.2, above.

6.1.2.4 Microbial Action

As discussed in Section 6.1.1.3, microorganisms are expected to consume oxygen, nitrogen and CO_2 and produce CO_2. They are also likely to consume nitrogen, fixing it as nitrate in water solution. The mass of bacteria present during the thermal period of the repository is expected to be very small (CRWMS M&O 1998). Before and after the thermal period, the mass of microorganisms will increase, but the flux of gas from the atmosphere through the rock mass will be very large compared to bacterial metabolism.

6.2 MASS-BALANCE CALCULATION

A mass balance calculation was performed to evaluate the effect of repository materials on the gases present in the drift over time. This calculation was similar to the calculation performed for the TSPA-VA, as described in Section 4.4.3 of that document (CRWMS M&O 1998), but is based on more recent design information and corresponding engineered material masses. The gas fluxes from the TSPA-VA are used as boundary conditions because of the lack of more recent information.

The calculational approach follows these steps: 1) the total mass of potential sinks is calculated for each gas, 2) the total moles of each potential sink is calculated by dividing the total mass by the appropriate atomic weight of each sink, 3) the equivalent amount (moles) of each gas consumed by those sinks is calculated using the appropriate stoichiometric factor, and 4) the amount of gas potentially consumed by the available sinks is compared to the amount of gas available in the drifts and the near-drift environment.

6.2.1 Carbon Dioxide

The potential sinks for CO_2 in or near the repository drifts are groundwater, cement associated with the rock bolts of the roof support, and the metal, which may possibly form carbonate compounds during corrosion. Interactions with materials in the rock are also possible; the most likely is dissolution of calcite resulting in increased CO_2 availability if acidic groundwater is formed, possibly as a result of corrosion.

The groundwater in the vicinity of the disposal drifts may act as a source or sink for CO_2, depending on pH and temperature. Solubility of CO_2 in groundwater increases as pH increases,

and decreases as temperature increases. During the thermal period, when gas influx is expected to be limited by production of water vapor, the solubility of CO_2 in nearby groundwater will be very low because of the limited amount of gaseous CO_2 available and because of the relatively low solubility of CO_2 in water at the expected temperatures. After ambient temperatures are reestablished, groundwater may be a source of CO_2 to the disposal drifts if other mechanisms act to remove CO_2 from the gas or liquid states. These mechanisms may include formation of secondary minerals in the rock as saturation is achieved, or the formation of metal carbonates during corrosion.

Approximately 91 kg of expansive cement (Portland Type k) per meter of drift is used to install rock bolts for roof support in approximately 30% of the drifts (CRWMS M&O 1999c). This grout will remove CO_2 from the gas in and near the drifts by carbonation of the calcium contained in the cement. The 91 kg/m of expansive cement (Portland Type k) used contains 45.4% Ca by weight (DTN: MO9909SPATYPEK.004), or 41.3 kg Ca/m. Dividing this by the atomic weight of Ca (40.08) (Weast, 1979) to convert to moles of Ca, the grout contributes 1,030 moles of Ca per each meter of drift where rock bolts are installed. This Ca will in turn consume an equivalent amount of CO_2 gas, which is assumed to proceed uniformly until all of the Ca in the cement has been converted to $CaCO_3$.

It is possible that metal carbonates, such as $FeCO_3$ (siderite), may form during corrosion. The extent to which this will occur depends on chemical conditions, primarily pH and temperature. The formation of carbonates must compete with formation of oxides, hydroxides, oxyhydroxides, sulfates, and more complex compounds. Equilibrium chemical modeling beyond the scope of this work, will be required to evaluate this process. At the present time, oxides and oxyhydroxides are expected to be the dominant corrosion products (CRWMS M&O 1999e, Section 6.5.1.1).

The TSPA-VA (CRWMS M&O 1998, p.4-45) gave the following discussion for the expected flux of CO_2 into the disposal drifts:

> "The model of air composition is implemented only as a logical model (there is not a code that calculates the values); the values are assigned directly for the specific periods in the system evolution. The oxygen and nitrogen values used are atmospheric, about 20 volume percent oxygen and 80 volume percent nitrogen, throughout all periods, except with the partial pressure of the nitrogen gas adjusted to 70 volume percent to offset the increased carbon dioxide in Period A. For carbon dioxide (as discussed in Sections 4.2.1.1.1 and 4.2.3.1.1) the ambient value is taken as 1,000 ppmv (parts-per-million by volume). A value of 100,000 ppmv, or 10 volume percent, is designated for the first 200 years (Period A) to reflect enhanced CO_2 in the gas possibly from either reaction of heated calcite and silica to form a calcium-silicate mineral, degassing of CO_2 from heated water, or release of carbon dioxide from the water-mineral interface (Section 4.2.3.1.1; Codell and Murphy 1992; Hardin et al. 1998, Section 5.7.1, 6.2.1, and 6.6). The abstracted air composition in terms of the carbon dioxide content through time to 10,000 years is shown in Figure 4-27. The initial transient period of enhanced carbon dioxide content shows up clearly."

The TSPA-VA (CRWMS M&O 1998, Section 4.6.2.1) used a cumulative mass flux of carbon dioxide from both the gas and water of about 51,300 moles of carbon dioxide per meter of tunnel through the drift over the first 100,000 years as a basis for its calculations. At 10,000 years, about 4,200 moles of carbon dioxide have passed through the drift, and the gas and water fluxes contribute about equally to this mass. The TSPA-VA found about 20,000 moles of Ca per meter of tunnel, based on a design with the drifts completely lined by concrete. The more recent design (CRWMS M&O 1999c) does not use a concrete drift liner; the only concrete used is grout for the

rock bolts in the 30% of the drifts needing support. This translates to an average of 300 moles of Ca per meter over the entire repository. This will consume about 7% of the CO_2 entering the drifts in the first 10,000 years based on the TSPA-VA gas fluxes (see Assumption 3). Although this is calculation does not take into account the current Site Recommendation (SR) design gas fluxes, this should not result in any noticeable change in gas composition in the tunnels, even in the drifts in the non-lithophysal tuff where rockbolts and grout will be used, and therefore should have no affect on groundwater chemistry and related processes.

6.2.2 Oxygen

A mass balance calculation was used to evaluate the possible effect of materials in the disposal drifts on the oxygen fugacity. The total amount of structural metal in the repository and the amount of corrosion resistant metal present were determined as shown in Section 4.1. This mass of metal was then converted to moles of metal. Because the dominant metal present is iron, 1.5 moles O_2 are consumed for each mole of metal present, as discussed below.

The primary mechanism for depleting oxygen from the in-drift gases is corrosion of the large masses of metal left in the repository at closure. In addition to the spent fuel waste and associated cladding and containers, a large amount of additional metal will be left in the drifts at closure. This additional metal makes up the rock support system, the support system for transporting and handling the waste packages, the supports upon which the wastes will rest, the drip shield protecting the wastes from direct contact from seepage, the invert supports, and miscellaneous other materials left behind after operations cease. While many metals will be present in addition to iron, the assumption that the entire mass of metal is iron results in a reasonable approximation of oxygen consumption in the mass balance calculation (see Assumption 1 in Section 5.1). This error introduced by this assumption will be very small (less than one order of magnitude) with respect to errors introduced by use of other simplifying assumptions.

There is a difference in the corrosion behavior of the various metals and alloys in the disposal drifts (CRWMS M&O 1999e, Section 6.5.2.1). A large amount of the steel, primarily used for rock support and infrastructure, is high-carbon mild steel or other easily corrodable materials such as copper conductors (1219 kg/m total material, equivalent to 21,800 moles/m, see Table 1, calculated from the total mass of metal from the table divided by the atomic weight of iron). This steel is expected to corrode rapidly in repository conditions. Other alloys, including a large amount of stainless steel and more exotic alloys associated with the waste packages (5776 kg/m equivalent to 103,400 moles Fe/m, see Table 2 in Section 4.1), will be much slower to corrode. The problem of estimating corrosion rates in the disposal drifts is discussed in *In-Drift Corrosion Products,* ANL-EBS-MD-000041 Rev 00 (CRWMS M&O 1999e).

> "The geochemical environment described in Section 6.2 will provide ample conditions for the corrosion of steels and alloys that may be emplaced in the repository. Most metals are out of equilibrium with the oxidizing environment in the unsaturated zone. These metals will react with water and available oxygen to produce corrosion products under the temperature conditions that are expected in the repository drift. Some of the materials and their elemental compositions that may be emplaced will be more resistant to corrosion (usually due to the formation of metal-oxide passivation films), while others may tend to corrode very rapidly especially in the presence of concentrated waters due to evaporation and boiling.

> The difficulty in predicting the alteration products lies in the fact that the chemistry of the near-field environment to a great extent will control the rates of corrosion. However, coupling the chemistry directly with explicit corrosion models is extremely difficult, as with all coupled processes in the EBS. Each component depends on the results of the other components, thus only first order approximations of this coupling phenomenon are possible with the modeling techniques that were employed in TSPA-VA near-field environment calculations (CRWMS M&O 1998a)."

The TSPA-VA (CRWMS M&O 1998, Section 4.6.2.1, DTN.MO9807MWDEQ3/6.001) assumed as a basis for its calculations that "a cumulative mass flux of oxygen from both the gas and water fluxes indicates that oxygen levels may be low during the peak boiling period (out to about 1,000 years). However, by 4,000 years the cumulative oxygen gas flux is up to about 1.7×10^5 moles of oxygen gas per meter of drift. Under these conditions, corrosion of all of the mild steel ($2.2\text{x}10^4$ moles Fe, calculated by dividing the total mass of metal by the atomic weight of iron) would consume only about $3.3\text{x}10^4$ moles of O_2, about 14% of the available oxygen during this period. The more corrosion-resistant metals (equivalent to $1.0\text{x}10^5$ moles of metal, $1.5\text{x}10^5$ moles of O_2) could also corrode to a lesser extent during this period without reducing the oxygen fugacity in the drifts enough to significantly alter the in-drift chemistry, that is, to change chemical conditions to the point that oxidation of metals is no longer the dominant corrosion mechanism. Note that this result is based on Assumption 3 and is not reflective of the SR gas fluxes.

7. CONCLUSIONS

7.1 SUMMARY OF BASIC CONCEPTS

The analysis discussed in this report provides the basis for constraining the values of the gas flux and composition in the potential emplacement drifts in terms of the major geochemical constituents carbon dioxide (CO_2,) oxygen (O_2), nitrogen (N_2), and steam or water vapor (H_2O). This work (1) develops a conceptualization of important processes affecting gas composition in the drift, and (2) uses mass balance considerations for the major potential sources and sinks of both oxygen and carbon dioxide to assess whether these may affect the gas composition within the drift relative to the composition and flux of these constituents entering the drift. The approach discussed in this document can be used for tracking gas composition in the drift relative to the incoming gas composition, as necessary for these constituents.

The gases expected to be of importance in system performance are the major gas constituents: steam (H_2O), oxygen (O_2), nitrogen (N_2) and carbon dioxide (CO_2). Water vapor will be primarily affected by thermal processes and it is not expected that chemical reactions will have any significant effect on its abundance in the repository. Nitrogen is potentially important to microbial communities in the repository, but geochemical reactions are not expected to have a significant impact on its abundance. The potential sources of in-drift gases include infiltration through the rock from the land surface, exsolution from groundwater, bacterial action, gas production from corrosion, radiolysis, and decay of radionuclides. Potential gas sinks identified include solution into groundwater, reaction with rock and repository engineered materials, displacement by other gases and vapors, and bacterial action. The rate of each of these processes varies as a function of repository conditions, and therefore varies with time and location within the drifts as the repository goes through heating and cooling over the first several thousand years after closure.

7.2 EXPECTED IMPACT ON IN-DRIFT CHEMICAL ENVIRONMENT

The conceptual analysis and mass balance calculations presented here suggest that in-drift gas flux and composition will not be strongly affected by interactions with in-drift and near-drift materials. However, in drift-gases will be displaced by steam during the thermal period, thus dropping the levels for all gases (except water vapor) in the drifts during that period. Even this decrease in oxygen fugacity is not expected to be great enough to reverse redox reactions occurring in the repository. The boundary conditions which use in-drift gas compositions and fluxes ignoring interactions with materials in and near the drifts will not be significantly changed by those interactions. These calculations are based on gas flux boundary conditions from the TSPA-VA, which are not expected to change significantly the findings of this analysis. The calculations presented here must be revisited when new boundary condition data become available.

7.3 EVALUATION OF NRC ISSUE RESOLUTION STATUS REPORT CRITERIA

As this documentation contains only conceptual discussions of the potential impacts on in-drift gases, not all of the criteria in Section 4.2 can be evaluated nor do they all apply at this time.

From Section 4.2.1.1 (Data and Model Justification Acceptance Criteria), criteria 4 and 5 do not apply, and criteria 3, 6 and 7 were not addressed and need further work. Only criteria 1 and 2 were addressed in this model.

From Section 4.2.1.2 (Data Uncertainty and Verification Acceptance Criteria), the five criteria apply to the use and selection of data used in the model and analysis. As the model for this activity will not be carried further in performance assessment, data uncertainty has not been addressed.

For Section 4.2.1.3 (Model Uncertainty Acceptance Criteria), the three criteria apply to the use and selection of data used in the model and analysis. As the model for these activities will not be carried further in performance assessment, the criteria are not addressed.

For Section 4.2.1.4 (Model Verification Acceptance Criteria), these criteria do not apply to the conceptual portions of the models and have not been addressed.

7.4 TBV IMPACT

The findings of this analysis are based on a number of TBV data and assumptions. The calculations discussed here must be revisited when qualified data, particularly design parameters describing repository materials and gas flux data from the Incoming Gas Model are available. While the data used in this report may be somewhat different in final form, the conclusion reached in this report is not sensitive to minor variations in those data. No quantitative results have been generated in this report.

This document may be affected by technical product input 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.

7.5 FEP'S EVALUATION

Although the issues found in Table 3 are discussed in this conceptual model, the issues cannot be fully resolved until repository modeling is completed as part of total system performance assessment.

8. REFERENCES

8.1 GENERAL REFERENCES

CRWMS M&O (Civilian Radioactive Waste Management Services Management and Operations) 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. *Provide Sub-models for the Physical and Chemical Environment Abstraction Model for TSPA-LA.* TDP-WIS-MD-000006. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990902.0450.

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

CRWMS M&O 1999c. *Request For Repository Subsurface Design Information To Support TSPA-SR.* Input Transmittal PA-SRR-99218.Ta. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990901.0312

CRWMS M&O 1999d. *YMP FEP Database Rev. 00C.* Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19991214.0518; MOL.19991214.0519.

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

CRWMS M&O 2000a. *Drift-Scale Coupled Processes (DST and THC Seepage) Models.* MDL-NBS-HS-000001 REV 00. Las Vegas, Nevada: CRWMS M&O. URN-0042.

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

CRWMS M&O 2000c. *Physical and Chemical Environment Model.* Input Transmittal 00224.T. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20000412.0789.

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

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

DOE (U.S. Department of Energy) 1998. *Total System Performance Assessment*. Volume 3 of *Viability Assessment of a Repository at Yucca Mountain*. DOE/RW-0508. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.19981007.0030.

Faure, G. 1986. *Principles of Isotope Geology*. 2nd Edition. New York, New York: John Wiley & Sons. TIC: 237212.

Walker, W.F. and Miller, D.G. 1984. *Chart of the Nuclides with Physical Constants, Conversion Factors, and Table Equilvalents*. Thirteenth Edition. San Jose, California: General Electric Company. TIC: 229820.

Weast, R.C., ed. 1979. *CRC Handbook of Chemistry and Physics*. 60th Edition, 1979 - 1980. Boca Raton, Florida: CRC Press. TIC: 245312.

8.2 CODES, STANDARDS, REGULATIONS, AND PROCEDURES

AP-SI.1Q, Rev. 2, ICN 4. *Software Management*. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.20000223.0508.

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.

Dyer, J.R. 1999. "Revised Interim Guidance Pending Issuance of New U.S. Nuclear Regulatory Commission (NRC) Regulations (Revision 01, July 22, 1999), for Yucca Mountain, Nevada." Letter from Dr. J.R. Dyer (DOE/YMSCO) to Dr. D.R. Wilkins (CRWMS M&O), September 3, 1999, OL&RC:SB-1714, with enclosure, "Interim Guidance Pending Issuance of New NRC Regulations for Yucca Mountain (Revision 01)." ACC: MOL.19990910.0079.

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

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.

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.

8.3 SOURCE DATA, LISTED BY DATA TRACKING NUMBER

MO9807MWDEQ3/6.001. Chapter 4 TSPA-VA Technical Basis Document Near-field Geochemical Environment. Eq3/6: In Drift Gas Model. Submittal date: 08/06/1998.

MO0001SPARSD38.014. Repository Subsurface Design ASTM Standard Material Compositions for Use in MING V1.0 TSPA-SR Calculations. Submittal date: 01/19/2000.

MO0003SPAARD38.026. Abstracted Repository Design Material Compositions used in TSPA-SR In Drift Microbial Communities Model Calculations. Submittal date: 03/22/2000

MO0003SPAARD38.023. Abstracted Repository Design Materials Quantities for use in TSPA-SR In Drift Microbial Communities Model Calculations Submittal date: 03/22/2000.

MO0001SPAAWP38.010. Abstracted Waste Package Design Materials Quantities for use in TSPA-SR In-Drift Microbial Communities Model. Submittal date: 01/19/2000. Submit to RPC URN-0239

MO0001SPAWPD38.009. Waste Package Design ASTM Standard Materials Compositions for use in TSPA-SR In Drift Microbial Communities Model Calculations. Submittal date: 01/19/2000.

MO0001SPACSS38.017. Composition of 316 NG Stainless Steel used in the In Drift Microbial Communities Model for TSPA-SR. Submittal date: 01/19/2000.

MO0001SPANEU38.018. Composition of Neutronit A987 Used in in Drift Microbial Communities Model for TSPA-SR. Submittal date: 01/19/2000. Submit to RPC URN-0238

MO9909SPATYPEK.004. Chemical and Mineralogical Compositions of Type K Cement. Submittal date: 09/14/1999.