OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
ANALYSIS/MODEL COVER SHEET

Complete Only Applicable Items

1. QA: QA

2. ☐ Analysis ☐ Engineering ☐ Performance Assessment ☐ Scientific	3. ☒ Model ☒ Conceptual Model Documentation ☐ Model Documentation ☐ Model Validation Documentation

4. Title:

In Drift Corrosion Products

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

ANL-EBS-MD-000041 Rev 00

6. Total Attachments:	7. Attachment Numbers - No. of Pages in Each:
1	I-11

	Printed Name	Signature	Date
8. Originator	Darren M. Jolley		12/2/99
9. Checker	Haywood Anderson		12/2/99
10. Lead/Supervisor	David Sassani		12/2/99
11. Responsible Manager	for Robert MacKinnon	E.L. Frankiewicz	12/2/99

12. Remarks:

This document is associated with AMR E0020

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
ANALYSIS/MODEL REVISION RECORD

Complete Only Applicable Items

2. Analysis or Model Title:

In Drift Corrosion Products

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

ANL-EBS-MD-000041 Rev 00

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

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
TECHNICAL CHANGE REQUEST

QA:

Section 1 - Change Description

1. TCR NO.: T1999 - 0181

1a. INTERIM TCR NO.: *(expedited changes only)*

2. PRIORITY: ☑ Routine ☐ Expedited

3. Q: ☑ Q ☐ Non-Q

4. DOCUMENT ACTION: ☑ Initial Issue ☐ Revision ☐ Change ☐ Editorial

5. TCR TITLE: In-Drift Corrosion Products

6. ORIGINATOR:

Name	Signature	Date	Phone	Bldg./Room
Darren Jolley		8/23/99	5-1661	1506M

7. DOCUMENTS REQUIRED TO IMPLEMENT CHANGE:

Document No. ANL-EBS-MD-000041 Rev./ICN 00

Title In-Drift Corrosion Products

☐ Continuation Page ____

8. TCR JUSTIFICATION:
This work is required to incorporate the following key issues into the EBS Physical and Chemical Environment Model: (1) drip shield and waste package chemical environments, (2) waste form chemcial environment, and (3) EBS transport pathway chemical environment

☐ Continuation Page ____

9. TCR DESCRIPTION: *(Include sketch(es) as necessary)*
To address these key issues, this work will develop a sub-model/analysis that accounts for the effects of corrosion products in the drift. Much of this work will be based on the methodology and sub-models developed for the TSPA-VA. This work is intended to address the review comments made during the production of the Viability Assessment Technical Basis Document and NRC IRSR (ENFE, CLST, TEF) criteria.

☐ Continuation Page ____

10. ATTACHMENTS:

☐ Continuation Page ____

11. RELATED CAUSE DOCUMENT(S): (TCR, CAR, NCR, DR, ETC.)
N/A

12. CAUSE CODE(s)
1. 25
2. ____
3. ____
4. ____

13. IMPACT IF CHANGE IS NOT MADE:
If this work is not performed, the following key issues will not be incorporated into the EBS Physical and Chemical Environment Model: (1) drip shield and waste package chemical environments, (2) waste from chemical environment, and (3) EBS transport pathway chemical environment.

☐ Continuation Page ____

14. RESPONSIBLE SUPERVISOR:

Name	Signature	Date/Time	Phone	Bldg./Room
Rob Howard		23 AUG 99 1:30pm	702-295-3097	15/1503

Section 2 - Disposition of Expedited Changes

	Name	Signature	Date	Concur?
15. SME:				☐ Yes ☐ No
16. QQA REPRESENTATIVE:				☐ Yes ☐ No
17. RESPONSIBLE MANAGER:				Interim Approval? ☐ Yes ☐ No

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
TECHNICAL CHANGE REQUEST

QA:

18. TCR NO.:	19. INTERIM TCR NO.: *(expedited changes only)*	20. ACCEPTED BY CCB SECRETARY:
T1999-0181		1. Initials ____ Date/Time ____ 2. Initials ____ Date/Time ____

Section 3 - Impact Analysis

21. DISPOSITION AUTHORITY: ☐ RM ☐ OM ☒ CCB

22. AUTHORIZATION TO CONTINUE: ☒ Yes ☐ No
JK CLARK — Name; Signature; 10/6/99 — Date

23. CCB REQUIRED REVIEW LIST CHANGE: ☐ Yes ☒ No

24. TECHNICAL IMPACT(S): ☐ N/A

	Yes	No		Yes	No		Yes	No
1. Design	☐	☒	5. Interface	☐	☒	9. Scientific Investigation	☐	☒
2. QA	☐	☒	6. Regulatory/Environmental	☐	☒	10. Specialty Engineering	☐	☒
3. Safety/Health	☐	☒	7. Construction	☐	☒	11. Affected Technical Documents	☐	☒
4. OMT	☐	☒	8. Waste Isolation	☐	☒	12. Performance Assessment	☐	☒
						13. Other	☐	☒

☐ Continuation Page ____

25 COST IMPACT(S): ☐ N/A

	Yes	No	Increase	Decrease	Amount
1. TPC	☐	☒	☐	☐	$ ____
2. TSLCC	☐	☒	☐	☐	$ ____
3. Budget Baseline:	☐	☒	☐	☐	$ ____

☐ Continuation Page ____

26. SCHEDULE IMPACT SCOPE:
☐ Level 0 ☐ Level 1 ☐ Level 2 ☐ Level 3 ☒ N/A
☐ Delay ☐ Improve ____ Days
☐ Continuation Page ____

27. OTHER IMPACTS: ☐ N/A

	Yes	No		Yes	No
1. Institutional	☐	☒	3. Programmatic	☐	☒
2. Contractual	☐	☒	4. Work Scope	☐	☒

28. OTHER IMPACTED DOCUMENTS: *(enter document no. & title)*

NONE

☐ Continuation Page ____

Section 4 - Disposition

29.

FUNCTION	RECOMMENDED? Yes	No	N/A	PRINT NAME/INITIAL/DATE	FUNCTION	RECOMMENDED? Yes	No	N/A	PRINT NAME/INITIAL/DATE
	☐	☐	☐			☐	☐	☐	
	☐	☐	☐			☐	☐	☐	
	☐	☐	☐			☐	☐	☐	
	☐	☐	☐			☐	☐	☐	
	☐	☐	☐			☐	☐	☐	
	☐	☐	☐			☐	☐	☐	
	☐	☐	☐			☐	☐	☐	
	☐	☐	☐			☐	☐	☐	
	☐	☐	☐			☐	☐	☐	
	☐	☐	☐			☐	☐	☐	

30. DISPOSITION:
☒ Approve ☐ Approve with Conditions ☐ Disapprove ☐ Endorse ☐ Defer

*** After Making Disposition, Please Return TCR Package to the CCB Secretary ***

31. COMMENTS/IMPLEMENTING ACTIONS/RATIONALE FOR DISPOSITION OTHER THAN APPROVE:

32. ACTION ITEMS: ☐ Yes ☐ No ☐ N/A

☐ Continuation Page ____

	Name	Signature	Date
33. RESPONSIBLE MANAGER:			
34. RESPONSIBLE OPERATIONS MANAGER:			
35. CCB CHAIRPERSON:	JK CLARK		12/15/99

AP-3.4Q Preliminary Impact Analysis
TCR No. T1999-0181
SME: Darren Jolley
Date: 9/9/99

TCR Title: In-Drift Corrosion Products
DI: ANL-EBS-MD-000041
Rev: 00

a) Potential impacts on design, site characterization, and performance assessment.

The objective of this document, given in section 8 of the TCR form, is to address the following key issues for incorporation into the EBS Physical and Chemical Environment Model including drip shield and waste package chemical environments, the waste form chemical environment and the EBS transport pathway chemical environment. No impacts to design, site characterization, and performance assessment are planned as a result of this analysis, however, further work may be identified and could be an initiating factor for additional effort in any one of these areas.

b) Potential impacts on internal or external interfaces.

The proposed analysis will require design input from WPO and EBSO to PA.

c) Identification of potentially impacted documents by contacting Engineering Document Control for a search of the Document Input and Reference Sheet database (not required for initial issue).

This TCR is for an initial issue of an AP-3.1OQ analysis.

Alternatives to the Proposed Analysis

There are no alternatives to the to the proposed analysis, in general. Analyses demonstrating that features, events, and processes (in this case the chemical processes that are affected by alloy corrosion) have to be conducted to meet not only 10 CFR63 requirements but NRC IRSR key technical issue resolution criteria.

Detailed Impact Analysis

TCR Title: In Drift Corrosion Products

TCR Number: T1999-0181

Responsible Manager: Robert MacKinnon (295-4738)

SME: Darren M. Jolley
Date: 12/6/99
Signature:

Kevin R. Harbert
Date: 12/9/99
Signature:

This document provides the conceptual framework for the in-drift corrosion products sub-model to be used in subsequent PAO analyses including the EBS physical and chemical model abstraction effort. This model has been developed to serve as a basis for the in-drift geochemical analyses performed by PAO.

The following provides the details of the impact analysis.

Technical Impacts:

1. Design. No impact. The document is a conceptual model for abstraction analyses for TSPA-SR, thus has no direct impact on design.
2. QA. No impact. Same reasoning as for #l.
3. Safety and Health. No impact. Plan does not address safety and health of project members.
4. Operations, Maintenance and Testing. No impact. The conceptual model does not affect operations, maintenance or testing activities. Only the analyses to be conducted as implementation of the conceptual model could have an impact.
5. Interface. No impact, Plans for incorporation of conceptual model into EBS PMR are complete
6. Regulatory/Environmental. No impact. The conceptual model is consistent with R&L activities identified in Repository Safety Strategy. Environmental is not involved in post-closure analyses.
7. Construction. No impact. The conceptual model has nothing to do with construction activities. It is a conceptual model for post-closure performance analyses.
8. Waste Isolation. No impact. Again, this is a conceptual model, not analyses or activities at the site, so the document involved in the change request has no impact on waste isolation.
9. Scientific Investigation. No impact. The document has no impact on scientific investigation because it just outlines the conceptual processes affecting in drift corrosion.

10. Specialty Engineering. No impact. The conceptual model is for analysis of post-closure performance, and as such has no impact on these activities.
11. Affected Technical Documents. No existing documents are impacted by this plan. The document is a conceptual model to be included in the future EBS PMR as an input as well as input into other analyses to be documented later in TSPA-SR.
12. Performance Assessment. No impact. The conceptual model helps clearly define the approach and method utilized for TSPA-SR, an activity already in the baseline.
13. Other. No.

Cost Impacts:

Budget Baseline. No impact to the budget Baseline, the work scope to implement this change is contained within the DOE approved Baseline.

TPC: No increase cost to the TPC (Total Project Cost) due to limited funding below the TPC.

TSLCC: No impact to TSLCC (Total System Life Cycle Cost). The TSLCC estimate is based on the MGR cost estimate contained in the Viability Assessment Report and Baseline Change Proposal (BCP)-00-99-0009, Incorporate License Application Design Selection (LADS) Enhanced Design Alternative (EDA) II into the YMSCO Project Baseline. The change does not represent changes to the criteria or design used for the Viability Assessment design basis (technical basis for the MGR cost estimate) or the LADS EDA II Report (technical basis for the LADS EDA II cost estimate).

Schedule Impacts:

Based on a review of the Integrated Project Schedule (IPS) and the Project Summary Schedule (PSS) there are no impacts to Level 0, 1, 2, or 3 milestones or to schedule activities because of this change.

Other Impacts:

1. Institutional. No impact. The document is a conceptual model for TSPA-SR and has no relation to the items identified in AP3.4Q for this check.
2. Contractual. No impact. As mentioned, the document is a conceptual model, has been in the approved baseline, and is covered under existing contractual arrangements.
3. Programmatic. No impact. The document does not require implementation of any management plans. The management structure and plan is already in place.
4. Work Scope. No impact. The document does not affect the baseline work scope, because it is just completion of work scope that was already in the baseline.

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1. PURPOSE

As directed by a written development plan (CRWMS M&O 1999a), a conceptual model for steel and corrosion products in the engineered barrier system (EBS) is to be developed. The purpose of this conceptual model 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 NRC Issue Resolution Status Report (IRSR) for the Evolution of the Near-Field Environment (NFE) Revision 2 (NRC 1999).

This document provides the conceptual framework for the in-drift corrosion products sub-model to be used in subsequent PAO analyses including the EBS physical and chemical model abstraction effort. This model has been developed to serve as a basis for the in-drift geochemical analyses performed by PAO. However, the concepts discussed within this report may also apply to some near and far-field geochemical processes and may have conceptual application within the unsaturated zone (UZ) and saturated zone (SZ) transport modeling efforts.

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, *Conduct of Activities*. The QAP-2-0 activity evaluation, *Activity Evaluation for 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 1998) requirements.

3. COMPUTER SOFTWARE AND MODEL USAGE

3.1 COMPUTER SOFTWARE

Software was not utilized in the development of this document

3.2 MODELS

The previous model used for PAO near-field geochemical analysis is documented in Chapter 4 of the Total System Performance Assessment-Viability Assessment (TSPA-VA) Analyses Technical Basis Document (TBD) (CRWMS M&O 1998a). This conceptual model document is being developed to supercede the concepts presented in the TBD document. This conceptual model eventually will become part of a new in-drift corrosion products model upon the completion of the appropriate input data and implementation documents and the completion of the GRIM V1.0 software code (CRWMS M&O 1999c). The old unqualified PAO near-field geochemical environment (NFGE) steel/corrosion model only is used in this document as a reference. The old model consists of the documentation found in Chapter 4 of the TBD

(CRWMS M&O 1998a), the use of EQ3/6 v7.2b software (CSCI: LLNL #: URCL-MA-110662 V7.2b) (Wolery 1992a, Wolery 1992b; Wolery and Daveler 1992), and the input and output files found in the following technical data management system (TDMS) Model Warehouse Data DTN MO9807MWDEQ3/6.000.

4. INPUTS

4.1 DATA AND PARAMETERS

For TSPA-Site Recommendation/License Application (SR/LA) analyses, requests were made by PAO to the Waste Package Operations (WPO), Engineered Barrier System Operations (EBSO) and Repository Subsurface Design Organization (RSDO) to obtain the appropriate information for the in-drift geochemical model analyses. Each organization responded using AP-3-14 *Transmittal of Input* to provide the requested information (CRWMS M&O 1999d, CRWMS M&O 1999e, and CRWMS M&O 1999f). Because these inputs are not all qualified or accepted they are considered TBV inputs. However, these inputs do contain some qualified and accepted data (e.g. reference to American Society for Testing and Materials [ASTM] standards).

4.1.1 Repository Drift Design Inputs

The Request for Repository Subsurface Design Information to Support TSPA-SR (CRWMS M&O 1999d) is the source of the information provided below. These inputs are synthesized in the following tables along with the appropriate assumptions (5.1, 5.2, 5.3, 5.4, and 5.5) found in section 5.

Table 1. Quantity and compositions of metals and alloys in an EDA II repository drift (excludes materials provided by the WPO organization listed in Table 2).

Material	Metal/Alloy	Quantity* (kg/m)	Composition (%)**							
			Fe	*Mn*	*Ni*	*Mo*	*Co*	*W*	*Cr*	*Cu*
Rock Bolt sets$	ASTM F432	48	99.022	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Welded Wire Fabric$	Steel	70	98.8	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Gantry Rail	ASTM A759	133.9	97.59	1.0	n/a	n/a	n/a	n/a	n/a	n/a
Rail Fittings$	Steel	13.4	74.44	n/a	n/a	n/a	n/a	n/a	n/a	25.0
Steel Sets$	ASTM A572	369	97.48	1.65	n/a	n/a	n/a	n/a	n/a	n/a
Conductor Bar Ftgs$.	ASTM A572	0.2	97.48	1.65	n/a	n/a	n/a	n/a	n/a	n/a
Communications Cable$	Copper	0.79	n/a	n/a	n/a	n/a	n/a	n/a	n/a	50.0
Conductor bar	Copper	5.32	n/a	n/a	n/a	n/a	n/a	n/a	n/a	100
Steel Invert$	ASTM A572	587	97.48	1.65	n/a	n/a	n/a	n/a	n/a	n/a
Loading Dock Steel$	ASTM A572	100	97.48	1.65	n/a	n/a	n/a	n/a	n/a	n/a

*Quantity refers to either a one-meter length of repository drift or a one-meter length of waste package depending on the materials listed. Additionally, the values reflect the ground support for the "nonlithophysal" portion of the repository drift design (CRWMS M&O 1999d). Note: wire conductor is not included as its relative abundance is small compared to remainder of materials. **The composition on this table does not reflect the entire composition of the metal or alloy, only the elements listed in the table. $See applicable assumption in Section 5.

4.1.2 Waste Package Design Inputs

The three input transmittals provided from waste package design (CRWMS M&O 1999e, 1999f, and 1999g) were reviewed and the data therein were tabulated and are presented in Table 2 below. Assumptions 5.6 and 5.7 were also used in the derivation of this table.

Table 2 Quantity and compositions of potential metals and alloys per meter of a 21 PWR waste package excluding waste form in the waste package.

Material	Metal/Alloy	Quantity* (kg/m)	Composition (%)**							
			Fe	*Mn*	*Ni*	*Mo*	*Ti*	*Al*	*Cr*	*B*
WP supports	ASTM B 575	267	6.0	0.5	50.015	14.5	n/a	n/a	22.5	n/a
WP supports	ASTM 316L	128	62.05	2.0	14.0	3.0	n/a	n/a	18.0	n/a
WP Outer Barrier[%]	ASTM B 575	1173	6.0	0.5	50.015	14.5	n/a	n/a	22.5	n/a
WP Inner Barrier[%]	ASTM 316NG	2106	62.06	2.0	14.0	3.0	n/a	n/a	18.0	n/a
Thermal Shunt	Al Type 6061	63	0.7	0.15	n/a	n/a	n/a	95.85	0.35	n/a
Absorber plates	Neutronit A 978	387	66.66	n/a	13.0	n/a	n/a	n/a	18.5	1.6[##]
Basket Guides	ASTM A 516	1073	97.91	1.3	n/a	n/a	n/a	n/a	n/a	n/a
Drip Shield	ASTM B 265 Grade 7[#]	563	0.3	n/a	n/a	n/a	98.665	n/a	n/a	n/a
Drip Shield	ASTM B 575	16	6.0	0.5	50.015	14.5	n/a	n/a	22.5	n/a

*Quantity refers to either a one-meter length of repository drift or a one-meter length of waste package depending on the materials listed. **The composition on this table does not reflect the entire composition of the metal or alloy, only the elements listed above. [#]Titanium composition also contains 0.25% Palladium (CRWMS M&O 1999g). [##]See Section 5 below for source of this value (CRWMS M&O 1999e). [%]The outer barrier is considered the corrosion resistant material (CRM) and the inner barrier is considered structural steel.

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 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.

4.2.1.1 Data and Model Justification Acceptance Criteria

1. Available 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 4.1.1, 4.2.1, 4.3.1, 4.4.1, and 4.5.1]

2. DOE's evaluation of coupled THC processes properly considered 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, 4.4.1, and 4.5.1]

3. Sufficient data were collected 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, 4.4.1, and 4.5.1]

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 4.1.1, 4.2.1, 4.3.1, 4.4.1, and 4.5.1]

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 4.1.1, 4.2.1, 4.3.1, 4.4.1, and 4.5.1]

6. Sensitivity and uncertainty analyses (including consideration of alternative conceptual models) were used 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, 4.4.1, and 4.5.1]

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, DOE has identified 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, 4.4.1, and 4.5.1]

4.2.1.2 Data Uncertainty and Verification Acceptance Criteria

1. Reasonable or conservative ranges of parameters or functional relations were used 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 4.1.1, 4.2.1, 4.3.1, 4.4.1, and 4.5.1]

2. Uncertainty in data due to both temporal and spatial variations in conditions affecting coupled THC effects on the chemical environment for radionuclide release were considered. [NRC (1999), Sections 4.1.1, 4.2.1, 4.3.1, 4.4.1, and 4.5.1]

3. DOE's evaluation of coupled THC processes properly considered 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 4.1.1, 4.2.1, 4.3.1, 4.4.1, and 4.5.1]

4. The initial conditions, boundary conditions, and computational domain used in sensitivity analysis involving coupled THC effects on the chemical environment for radionuclide release were consistent with available data. [NRC (1999), Sections 4.1.1, 4.2.1, 4.3.1, 4.4.1, and 4.5.1]

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, 4.4.1, and 4.5.1]

4.2.1.3 Model Uncertainty Acceptance Criteria

1. Appropriate models, tests, and analyses were used 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 4.1.1, 4.2.1, 4.3.1, 4.4.1, and 4.5.1]

2. Alternative modeling approaches consistent with available data and current scientific understanding were investigated, and their results and limitations were appropriately considered. [NRC (1999), Sections 4.1.1, 4.2.1, 4.3.1, 4.4.1, and 4.5.1]

3. DOE provided 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 4.1.1, 4.2.1, 4.3.1, 4.4.1, and 4.5.1]

4.2.1.4 Model Verification Acceptance Criteria

1. The mathematical models for coupled THC effects on the chemical environment for radionuclide release are 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, 4.4.1, and 4.5.1]

2. DOE appropriately adopted 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, 4.4.1, and 4.5.1]

3. Abstracted models for coupled THC effects on the chemical environment for radionuclide release are based 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 4.1.1, 4.2.1, 4.3.1, 4.4.1, and 4.5.1]

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 1999i) 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

No codes were used in this document.

4.3.2 Standards

ASTM C 1174-97 *Standard Practice for Prediction of the Long-Term Behavior of Materials, Including Waste Forms, Used in Engineered Barrier Systems (EBS) for Geological Disposal of High-Level Radioactive Waste* was used as guidance in the preparation of this conceptual model.

The following standards were used in the preparation of this document (The references are included in Section 8.2).

- ASTM A572
- ASTM A759
- ASTM F432

5. ASSUMPTIONS

5.1. The steel in rail fittings is ASTM A572 steel. No material type was designated in CRWMS M&O (1999d), therefore this composition is deemed a reasonable alternative due to the fact that mild carbon steels have generally the same compositions. The 13.4 kg/m of steel is also the 75%-25% mixture of steel and copper, not just the steel. This is made to clarify the ambiguity in the reference (CRWMS 1999d) [used in Section 4.1.1 and 6.4]

5.2. The steel in conductor bar fittings is ASTM A572 steel. No material type was designated in CRWMS M&O (1999d), therefore this composition is deemed a reasonable alternative due to the fact that mild carbon steels have generally the same compositions [used in Section 4.1.1 and 6.4].

5.3. The reference to trace quantities of associated metals and halides was not included in the compositions reported in ASTM F432, ASTM A759 and ASTM A572 because their actual compositions are not known and their abundance is small and would not impact this evaluation [used in Section 4.1.1 and 6.4].

5.4. A combination of the heat and product composition values for C, S, and P was used from compositions found in ASTM F432 for rock bolts. This is done to maximize the compositions of these elements so that the performance assessment models are bounded on the conservative side [used in Section 4.1.1 and 6.4].

5.5. Only 0.15% Vanadium was used for alloy compositions of ASTM A572 steel and nitrogen or columbium was not considered due to the limited abundance of these two materials in the standard composition (ASTM A572) [used in Section 4.1.1 and 6.4].

5.6. The boron content of Neutronit A-978 is assumed to be 1.6% as documented in CRWMS M&O (1999e) [used in Sections 4.1.2 and 6.4].

5.7. The materials in a 21 PWR waste package essentially bound the masses and types of materials that are to be used in the construction of all other waste packages (e.g. 44 BWR, DHLW, and Naval SNF) as materials used in waste package construction are similar in mass and composition (CRWMS M&O 1999f) [used in Section 6.4].

5.8. The elements found in the metals and alloys proposed in the enhanced design alternative (EDA) II design (CRWMS M&O 1999h) from a one meter segment of drift having a composition of greater than or equal to 1% will be included in the discussion in detail. All other elements are expected to have little or no impact on the bulk EBS geochemical environment due to their limited abundance [used in Section 6.4]

6. ANALYSIS/MODEL

6.1 PREVIOUS WORK

The conceptual model documented below and to be implemented in other document(s) that will be developed improves upon and supercedes the previous model used in TSPA-VA in-drift geochemical analyses (CRWMS M&O 1998a). The superceded model consisted of a simplifying assumption and an equilibrium calculation using the EQ3 software code (CRWMS M&O 1998a, Section 4.4.3.2.1). The simplifying assumption was that most of the water contacts corrosion products along the pathway into a breached waste package. The corrosion products were represented by the mineral goethite. The EQ3 calculation equilibrated the incoming water entering the breached waste package with goethite.

The TSPA-VA model (CRWMS M&O 1998a, Section 4.4.3.2.1) used Fe as the basis for the types of corrosion products being generated, thus the full compositions of the alloys and steels were neglected. Additionally there was no ability to quantify corrosion products through time; in other words, there was no tie-in to expected corrosion rates. The model documented below is the first step at improving the model documented in the TSPA-VA (CRWMS M&O 1998a, Section 4.4.3.2.1). It documents the geochemical system and the expected interactions of the introduced steels and alloys in both the ambient and perturbed geochemical environment.

6.2 INTRODUCTION TO THE GEOCHEMICAL SYSTEM

Below is a brief discussion of the ambient chemical system that this conceptual model is based on. The system includes two other general components along with the ambient geochemical system, namely the thermally perturbed system and the introduced materials. These three components of the system will control the alteration of the steels and alloys in the system and govern the formation of corrosion products. The interaction of the corrosion products with the waters that have come in contact with the waste form and are exiting the drift will in turn have great influence on the amount and type of radionuclides that are released from the engineered barrier system into the realm of the unsaturated zone flow and transport models. Sections 6.2.1, 6.2.2 and 6.2.3 below were taken from CRWMS M&O (1998a) that discussed the same issues. Changes were made to the text where necessary to reflect the current reference section listed in this document.

6.2.1 Ambient System

The discussion below provides general background on the geochemistry of the ambient system. A detailed review of this information has been conducted and is presented in the *Yucca Mountain Site Description* (CRWMS M&O 1998b, CRWMS M&O 1998e, and CRWMS M&O 1998f).

6.2.1.1 Gas Compositions

The abundance of the gases O_2, N_2, and Ar in samples of pore gases from the UZ are all very close to their atmospheric values (CRWMS M&O 1998b, Section 6.2.7.2, pp. 6.2-40). 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 parts-per-million-by-volume [ppmv]) by about a factor of three (CRWMS M&O 1998b, 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 1998f, 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 1998f, Section 5.3.4.2.4.6, p. 5.3-173).

6.2.1.2 Water Compositions

Analyses of the groundwater compositions at Yucca Mountain are described in detail in the *Yucca Mountain Site Description* (CRWMS M&O 1998f, Sections 5.3.4 and 5.3.5, and CRWMS M&O 1998b, Section 6.2). The ambient water composition could be defined either by analyzed values of saturated-zone water (e.g., Well J-13) or from the analyses performed on pore water extracted from UZ rock samples. Harrar et al. (1990) evaluated water from Well J-13 for use as a reference water composition and concluded that it could be used as such for the purpose of a reference case fluid. It was noted that fluids taken from flowing fractures at Rainier Mesa had compositions similar to the J-13 values (Harrar et al. 1990). The average composition of J-13 water from Harrar et al. (1990) is given in Table 4, together with averages for UZ fluids analyzed from boreholes UE-25 UZ-5 and UE-25 UZ-4 (Yang et al. 1988, Yang et al. 1990; Yang 1992).

Measurements of groundwater compositions from the SZ indicate that the fluids within the tuffaceous units (as represented by samples from well J-13) are predominantly dilute sodium bicarbonate fluids with high concentrations of aqueous silica (Benson et al. 1983; Ogard and Kerrisk 1984; Kerrisk 1987, Appendix B; Harrar et al. 1990). In general, the saturated-zone fluids have pH in the range of 7-8 (but cover 6.7 to 9.4), contain, in order of decreasing concentration, the additional cations Ca^{2+}, K^{+}, and Mg^{2+}, and the additional anions $SO_4^{2\&}$, $Cl^{\&}$, $F^{\&}$, and $NO_3^{\&}$. The groundwater from the deep Paleozoic carbonate aquifer (from UE&25p#1) is more highly concentrated with respect to all these constituents except aqueous silica and is characterized by pH values slightly lower than 7 (Ogard and Kerrisk 1984; Kerrisk 1987, Appendix B). The saturated-zone water analyses suggest that these fluids are, in general, relatively oxidized, but a couple of samples may indicate reducing conditions at depth (Ogard and Kerrisk 1984). A series of measurements of the saturated-zone system are underway to more fully determine the oxidation potential near the surface of the water table and as a function of depth into the aquifer. Measurements of the organic content of the saturated-zone fluids are below 1 ppm (Means et al. 1983).

Analyzed water compositions from the UZ tuffaceous rocks (Yang et al. 1988, Yang et al. 1990; Peters et al. 1992; Yang 1992) indicate that they have pH values in the range of 6.4 to 7.5 and that some constituents (Ca^{2+}, K^{+}, Mg^{2+}, $SO_4^{2\&}$, $Cl^{\&}$, and dissolved silica) are more concentrated than found in samples from the SZ tuffaceous aquifer. However, the average $HCO_3^{\&}$ content measured in 83 water samples extracted from UZ nonwelded tuff was lower than that in the

saturated-zone samples (Peters et al. 1992). Some of this variability may be caused by the extraction techniques used to remove water from unsaturated samples (Peters et al. 1992). No analyses of the dissolved organic content have been given in the studies of the UZ fluid compositions. Because of the intimate contact between the UZ fluids and the pore gases in the rock, these groundwaters are relatively oxidizing and the oxidation potentials are probably controlled primarily by atmospheric oxygen levels (CRWMS M&O 1998b, Section 6.2.5.2, p. 6.2-19). In the units above the Calico Hills, the pH of the water is thought to be dependent primarily on the carbon dioxide content of the gas, with some degree of Na^+-H^+ ion exchange affecting the values (CRWMS M&O 1998b, Section 6.2.5.2, p. 6.2-19).

Table 4. Average Chemistries for Saturated Zone Water Well (J-13) and for Unsaturated Zone Water (UZ-5 and UZ-4) (nr = not reported). Table taken from CRWMS M&O (1998a).

Constituent	Units	J-13 AVG[a]	UE-25 UZ-5 AVG[b]	UE-25 UZ-4 AVG[c]
Ca	mg/l	12.9	45.2	99.2
Mg	mg/l	2.0	9.2	17.4
Na	mg/l	45.8	39.1	56.4
K	mg/l	5.0	8.6	14.2
SiO_2	mg/l	61.0	92.4	86.8
NO_3^-	mg/l	8.8	nr	nr
HCO_3^-	mg/l	128.9[d]	nr	nr
Cl	mg/l	7.1	53.2	94.0
F	mg/l	2.2	nr	nr
SO_4^{2-}	mg/l	18.4	51.0	151.8
Li	microg/l	48.3	nr	nr
Fe	microg/l	~30	49.1	24.3
Mn	microg/l	~45	18.5	38.6
Sr	microg/l	~50	422.6	1196.5
Al	microg/l	~30	nr	nr
Zn	microg/l	nr	62.0	102.1
field Eh	mV	340.0	nr	nr
field O_2	mg/l	5.6	nr	nr
field pH	pH	7.4	7.0	7.5

[a]Averages from Harrar et al. (1990), note that approximate values are estimates based on few data in Harrar et al. (1990).

[b]Averages of data in Yang et al. (1988) and Yang et al. (1990).

[c]Averages of data in Yang et al. (1988) and Yang (1992).

[d]Alkalinity as HCO_3^-.

There are clearly differences between the J-13 and UZ fluids, primarily higher Ca, Mg, Cl, and $SO_4^{2\&}$ in the UZ fluids (see Table 4 above and discussion in CRWMS M&O 1998b, Section 6.2.5.2). Whether these differences are meaningful, as well as which fluid composition most closely represents the ambient composition of fluid that moves through Yucca Mountain is not currently completely understood. There may have been some alteration of UZ pore fluid chemistry from the extraction techniques, as discussed above. In addition, it was thought that the

UZ-4 samples had lost water by evaporation, which may account for the generally higher values compared to UZ-5 analyses (Peters et al. 1992; Yang 1992). Because of low sample volumes, the UZ analyses are not as comprehensive as those for the SZ. In addition, the saturated-zone fluids are similar compositionally to both the perched water (CRWMS M&O 1998b, Section 6.2.5.2, p. 6.2-19) and to that collected flowing from fractures at Rainier Mesa (Harrar et al. 1990, pp. 6.5 and 6.6, Table 6.1). At this time, it appears that a reasonable ambient water composition moving through fractures can be represented by the J-13 composition.

6.2.2 Introduced Materials

During both site characterization activities and the construction of a repository, a number of substances will be introduced into the site such that they become committed to remain in the system over geologic time. These may include a variety of compounds but there are three main categories that, as part of the waste package or as structural components, will potentially be abundant post-closure: steels and alloys, organic substances, and cementitious materials. This conceptual model's focus is on the steels and alloys that will be introduced into the drift environment.

Reaction of water with steel and alloys (much of which is iron [Fe], although other components are present in abundance in many alloys, including titanium, [Ti], chromium [Cr] and nickel [Ni]) in the potential drifts will liberate metal cations to the aqueous phase. The introduced material certainly increases the source mass for Fe and other metals in the system and could increase the concentration of dissolved Fe and other metal cations in the fluids. The natural groundwaters are relatively poor in dissolved metals, and the analyzed values probably represent colloidal material (Harrar et al. 1990). The major lithologies at the site in the potential repository horizon are felsic tuffs that contain about 1 to 3 percent total iron oxide, representing a relatively low Fe content for igneous rocks (Lipman et al. 1966; CRWMS M&O 1998e, Section 3.5).

The alteration of steels and alloys will produce metal-oxide and -hydroxide corrosion products within the drift and may form metal-silicate minerals. As the 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. Such oxidation reactions represent a source of metabolic energy for microbial activity within the potential emplacement drifts. The corrosion products will alter the sorptive properties of the EBS and affect transport of radionuclides within the drift. Colloids generated from steel and alloy corrosion products that strongly sorb radionuclides could provide additional radionuclide transport capabilities (Meike and Wittwer 1993; Triay et al. 1995). Because of the planned use of large amounts of steel and alloys in the potential repository, these types of colloids could have a large source capacity relative to the natural iron-oxyhydroxide colloids fluxing through the drift.

6.2.3 The Thermally Perturbed System

Water entering the drift that is available to interact with the steel and alloys will have a variable composition as a function of time as a result of the heating of the system driving processes such as boiling/condensation and reaction of both heated and condensate waters with minerals and gases in the fractures of the host rocks (Arthur and Murphy 1989; Glassley 1994; Murphy 1993; Wilder 1996; Lichtner and Seth 1996; Glassley 1997; Hardin et al. 1998, Section 6.2.2). These

reacted, or thermally perturbed, fluid compositions may flow down fracture pathways and enter potential emplacement drifts where they could undergo reaction with introduced materials or be boiled again and deposit mineral precipitates containing salts (Glassley 1994; Murphy and Pabalan 1994; Wilder 1996; Lichtner and Seth 1996). The total amounts of salts deposited within the drifts will depend to some extent on the composition of ambient water within the UZ.

As temperature increases, a number of changes may impact the geochemical behavior of the near-field environment. Mineral stabilities and phase equilibria are temperature dependent, and the rates at which reactions occur will generally increase at higher temperatures. Both continuous reactions such as the gradual dehydration or shift in cation composition of a solid phase, and discontinuous reactions such as the disappearance of a phase outside of its stability range, will occur as temperature increases (Glassley 1994; Murphy 1993; Hardin et al. 1998, Sections 5 and 6). The higher temperatures in the near-field may result in regions where attainment of thermochemical equilibrium can be assumed (Glassley 1994). Mineral transformation reactions, as well as precipitation/dissolution reactions will cause changes in porosity and permeability of the system as temperature increases (extending out into the geosphere—see Sections 5.6 and 5.7 in Hardin et al. 1998) and will result in a change in both the type and distribution of minerals present in the near-field (Glassley 1994; Wilder 1996).

The extent to which these effects may reach into the geosphere is illustrated by the potential extensive alteration of the basal vitrophyre of the Topopah Spring tuff with concurrent large changes in calculated porosity (Wilder 1996; Hardin et al. 1998, Sections 5.6 and 5.7). Such changes may impact the hydrologic properties of the system as well as the near-field and geosphere transport properties. The increased temperatures will vaporize much of the water in the near-field as an above-boiling temperature zone forms in the very near-field (Glassley 1994). This transition will increase the capacity of the system to transport moisture as volatiles and will result in precipitation of all dissolved solids from boiling fluids in the near-field. Condensation of steam as water in cooler regions above the potential repository horizon will dissolve new material, which could be transported through fractures back down into the boiling zone with subsequent boiling and phase precipitation. This refluxing could produce porosity and permeability changes that may impact the near-field hydrology (Glassley 1994; Hardin et al. 1998, Section 5.6).

Because boiling of fluids will occur, mineral precipitates including salts will form in the region of boiling. Water undergoing boiling/evaporation or reacting with precipitated salts will become concentrated in a number of dissolved constituents either in close proximity to, or within, potential emplacement drifts (Hardin et al. 1998, Section 6.2.2). Such fluids represent a second end-member for reaction with the EBS. Currently these fluid compositions are primarily constrained by the results of geochemical mass-transfer calculations for simplified systems designed to simulate the evaporation/boiling that would occur within a thermally perturbed repository environment. Results from two such calculations (Murphy and Pabalan 1994; Wilder, 1996; Hardin et al. 1998, Section 6.2.2) are discussed below.

In one calculation (Wilder 1996; Hardin et al. 1998 Section 6.2.2), ~J-13 water evaporates/boils along a temperature rise from ambient to 95°C at equilibrium with atmospheric gases. These calculations represent 95 percent evaporation. The second set of calculations (Murphy and Pabalan 1994) starts with model water evolved at 75°C (heated J-13 water that has reacted with

tuff), heats it instantaneously to 100°C in equilibrium with atmospheric oxygen and the calculated CO_2 fugacity. (This latter parameter value is higher than atmospheric values and was derived from a coupled reactive transport calculation in which both gas and fluid flow were calculated.) The compositions resulting from this second set of calculations are given up to about 99.6 percent evaporation. Even though the results of these two calculations are not directly comparable (because they represent different compositional systems and different controls on the gas phase), they appear to be roughly consistent. Relative to ambient compositions, these fluids have, in general, high ionic strength (greater than 1 molal stoichiometric ionic strength for the 99.6 percent evaporated case), are enriched in alkalis, chloride, sulfate, and other ligands (F^-, and HCO_3^-), and have higher pH (~9.5).

Because mineral precipitation occurs throughout these calculations (calcite, silica polymorphs, etc.), these compositions do not represent simply concentrated ambient values, but are selectively concentrated. In both sets of calculations, the dissolved Ca content is low (<50 mg/kg) because calcite precipitation depletes the fluid of Ca. However, other elements that are conservative within the aqueous phase are orders of magnitude higher than at ambient conditions. For example, at the 99 percent and 99.6 percent evaporation points, chloride concentrations are about 100-times and about 250-times higher, respectively, than the average value for J-13 water (Murphy and Pabalan 1994).

Modeling results for water evaporation indicate that the resultant composition may be profoundly affected by the gas phase assumed to be in equilibrium with the evaporating water—i.e., whether the system behaves as open to the atmosphere or in a closed manner (Wilder 1996; Hardin et al. 1998, Section 6.2.2). In equilibrium with the atmosphere gas, initial ~J-13 water evolves to higher pH (>9.5) and lower Eh (~+500 mV) at high degrees of evaporation, compared to the case where the system is isolated from the atmosphere for which the final values are pH < 6.8 and Eh > +650 mv. The model results are very sensitive to the constraints on CO_2 fugacity (Murphy and Pabalan 1994), with different solid phases precipitating for lower CO_2 fugacities. These results emphasize the need to have a model that incorporates consistently the evolution of near-field gas composition, and the need to have such constraints defined for each scenario.

The thermally driven perturbations to the system will also affect the flux and composition of gas entering the potential emplacement drifts (Murphy 1991; Glassley 1994; Codell and Murphy 1992; Murphy and Pabalan 1994; Lichtner and Seth 1996; Wilder 1996; Glassley 1997; Hardin et al. 1998, Section 5.7.1). One major process affecting the in-drift gas composition is the boiling of the pore water, which is expected to drive out most of the air component of the gas from the drift environment (Murphy 1991; Pruess et al. 1990a, Pruess et al. 1990b; Murphy and Pabalan 1994; CRWMS M&O 1997, CRWMS M&O 1998d). The changes in the air mass-fraction of the gas will drive changes in the water chemistry and changes to the solid materials in the drifts because of, for example, the interaction of CO_2 gas with (a) water in terms of pH controls, and (b) cementitious materials in terms of calcite formation and neutralization of alkalinity. These interactions between the water, the carbon dioxide, and the introduced materials may play a key role in determining some of the major chemical conditions of the thermally perturbed system.

6.3 LOCATIONS OF METALS/ALLOYS IN THE DRIFT

Figure 1 below shows the general locations of most of the EDA II design materials within a repository drift. For the site recommendation design the metals/alloys can be found in one of six locations: namely, (1) the ground support system, (2) the drip shield, (3) the waste package, (4) the waste package internal components (5) the pedestal and pier system, and finally (6) the invert.

6.4 COMPOSITIONS OF METALS IN THE DRIFT

Tables 1 and 2 document the quantities and compositions of the metals used in the EDA II design for a 21 PWR waste package. Additional information shown on the bottom two lines of Table 5 below was calculated and added to Table 1 to create Table 5. The same process was used to calculate the values at the bottom of Table 6. Two simple calculations were done to derive the additional data from the information found on Tables 1 and 2. First, to determine the mass of each element listed, the mass of each material was multiplied by the composition percentage and the resulting values were summed for each element. Second, the percent of the total mass was calculated by taking the sum of the total elemental mass and dividing it by the total mass of steel or alloy and multiplying by 100.

Of the 12 elements listed in Tables 1 and 2, there are several that are or could be present in quantities less than 1% over a meter of the repository drift. These are Pd, Co, W, B, and Cu. Because these are such low quantities and because of the uncertainties associated with any bulk geochemical calculation, a simplifying assumption is included where the elements discussed below in the conceptual model are based only on the elements at concentrations at or greater than 1% of the total metals/alloys found in a one meter segment of a repository drift (see assumption 5.8 above). Based on assumption 5.8, the following elements will be discussed below: Fe, Mn, Ni, Mo, Cr, Ti, and Al. Additionally, the results found on the following two tables (Table 5 and Table 6) should be considered TBV, due to unqualified inputs.

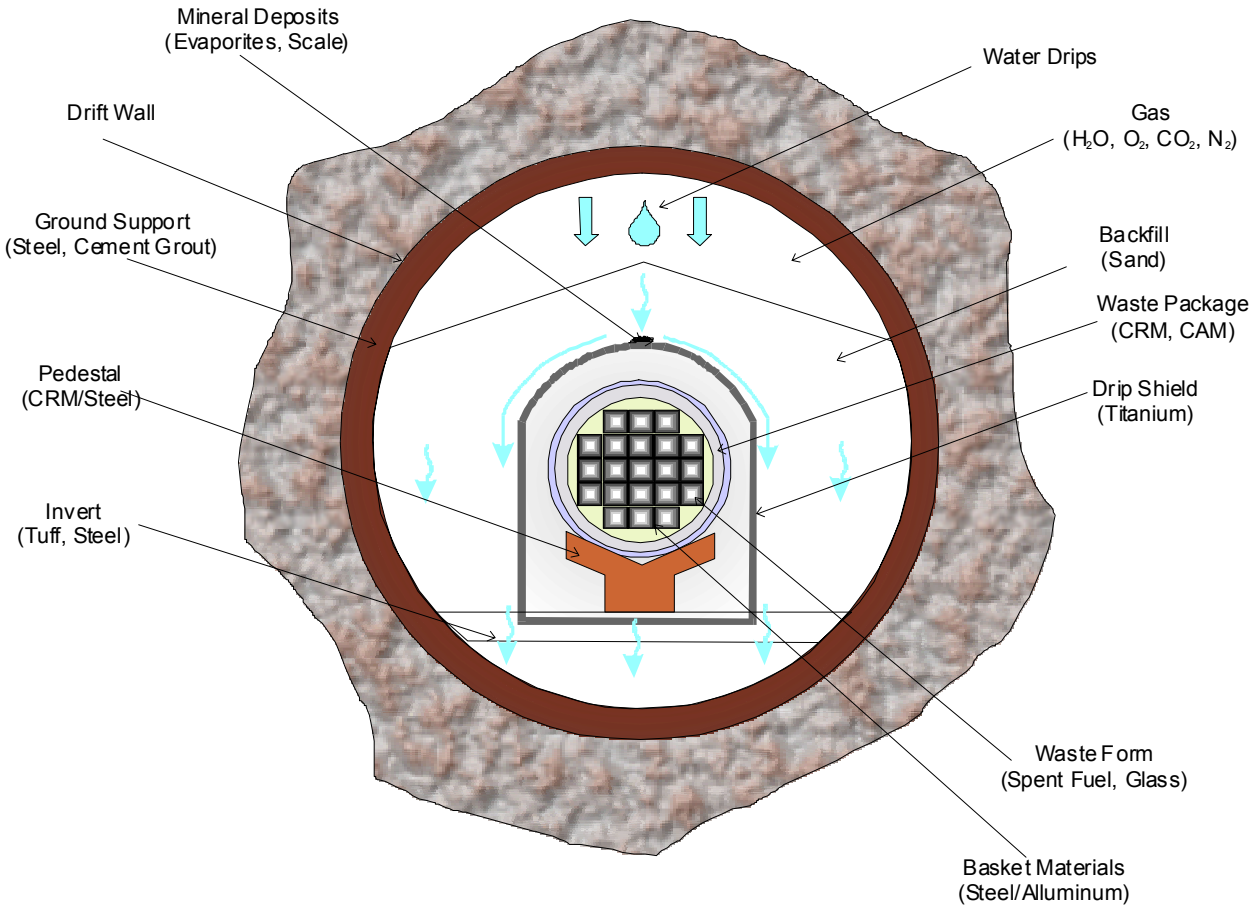

Figure 1. Conceptual description of the potential in-drift geochemical processes and the interaction with the materials of the EDA II design (this figure does not depict the rail and gantry systems from EDAII).

Table 5. Total masses and percentages of metals/alloys in a meter segment of repository drift based on the EDA II design (results based on Table 1 input and calculation documented in Section 6.4).

Material	Metal/Alloy	*Quantity (kg/m)	**Composition (%)							
			Fe	*Mn*	*Ni*	*Mo*	*Co*	*W*	*Cr*	*Cu*
Rock Bolt sets	ASTM F432	48	99.022	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Welded Wire Fabric	Steel	70	98.8	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Gantry Rail	ASTM A759	133.9	97.59	1.00	n/a	n/a	n/a	n/a	n/a	n/a
Rail Fittings/Copper	Steel	13.4	74.44	n/a	n/a	n/a	n/a	n/a	n/a	25.0
Steel Sets	ASTM A572	369	97.48	1.65	n/a	n/a	n/a	n/a	n/a	n/a
Conductor Bar Ftgs.	ASTM A572	0.2	97.48	1.65	n/a	n/a	n/a	n/a	n/a	n/a
Communications Cable	Copper	0.79	n/a	n/a	n/a	n/a	n/a	n/a	n/a	50.0
Conductor bar	Copper	5.32	n/a	n/a	n/a	n/a	n/a	n/a	n/a	100
Steel Invert	ASTM A572	587	97.48	1.65	n/a	n/a	n/a	n/a	n/a	n/a
Loading Dock Steel	ASTM A572	100	97.48	1.65	n/a	n/a	n/a	n/a	n/a	n/a
Total (kg/m)		1327.61	1286.92	18.77	n/a	n/a	n/a	n/a	n/a	9.07
% of Total mass			96.94	1.41	n/a	n/a	n/a	n/a	n/a	0.68

*Quantity refers to either a one-meter length of repository drift or a one-meter length of waste package depending on the materials listed. Additionally, the values reflect the ground support for the nonlithophysal repository drift design (CRWMS M&O 1999d). **The composition on this table does not reflect the entire composition of the metal or alloy, only the elements listed above.

Table 6. Total masses and percentages of metals/alloys within in a meter segment of a 21 PWR waste package based on the SR design (results based on Table 2 input and calculation documented in Section 6.4).

Material	Metal/Alloy	*Quantity (kg/m)	**Composition (%)							
			Fe	*Mn*	*Ni*	*Mo*	*Ti*	*Al*	*Cr*	*B*
WP supports	ASTM B 575	267	6.0	0.5	50.015	14.5	n/a	n/a	22.5	n/a
WP supports	ASTM 316L	128	62.05	2.0	14.0	3.0	n/a	n/a	18.0	n/a
WP Outer Barrier	ASTM B 575	1173	6.0	0.5	50.015	14.5	n/a	n/a	22.5	n/a
WP Inner Barrier	ASTM 316NG	2106	62.06	2.0	14.0	3.0	n/a	n/a	18.0	n/a
Thermal Shunt	Al Type 6061	63	0.7	0.15	n/a	n/a	0.15	95.85	0.35	n/a
Absorber plates	Neutronit A 978	387	66.66	n/a	13.0	n/a	n/a	n/a	18.5	1.6
Basket Guides	ASTM A 516	1073	97.91	1.3	n/a	n/a	n/a	n/a	n/a	n/a
Drip Shield	ASTM B 265 Grade 7	563	0.3	n/a	n/a	n/a	98.655	n/a	n/a	n/a
Drip Shield	ASTM B 575	16	6.0	0.5	50.015	14.5	n/a	n/a	22.5	n/a
Total (kg/m)		5776	2784.45	66.00	1091.29	278.14	555.52	60.39	801.53	6.19
% of Total mass			48.20	1.14	18.89	4.82	9.62	1.05	13.88	0.11

*Quantity refers to either a one-meter length of repository drift or a one-meter length of waste package depending on the materials listed. **The composition on this table does not reflect the entire composition of the metal or alloy, only the elements listed above.

6.5 CONCEPTUAL MODEL

6.5.1 Geochemistry of Metals in the Drift

For each of the seven elements selected (Fe, Mn, Ni, Mo, Cr, Ti and Al) there follows a brief discussion of the aqueous geochemical processes that control the solubility, dissolution, precipitation, oxidation and adsorption of these elements.

6.5.1.1 Iron (Fe)

Iron in the natural environment exists in two oxidation states. Fe(II) is the soluble form and is stable in the pH <6 range of natural waters. Fe(III) primarily forms insoluble oxides and oxyhydroxides (e.g. Fe_2O_3 and FeOOH respectively), its solubility product ranges from 10^{-39} to 10^{-44} at a pH >3 (Schwertmann and Taylor 1989, p. 381 and 396) and it is increasingly more soluble with lower pH (Pankow 1991, p. 231).

Table 7 shows the typical oxidation-reduction reactions of aqueous iron and the minerals they form. Figure 2 shows the formation of goethite (FeOOH) at the relatively high oxidation potentials expected at Yucca Mountain, however goethite may not be the stable phase over times of interest (on the order of years, decades and centuries). The stability of iron hydroxides and oxyhydroxides proceeds from amorphous $Fe(OH)_3$ to goethite to hematite [Fe_2O_3] at 25°C (Stumm and Morgan 1981, p. 434). Determining the stable phase between the goethite and hematite is much more difficult as the reaction from goethite to hematite is very slow (Krauskopf 1979, p. 208). However in soils, goethite tends to form under low temperatures (in cool or temperate climate zones), high H_2O activity and higher organic matter contents. The hematite-to-goethite ratio usually increases with increasing soil temperature (Schwertmann and Taylor 1989, pp. 398-400). pH also plays a role in the favorablity of the two phases. Goethite is favored in soils with low pH (3-7), whereas hematite is favored above pH 7 (Schwertmann and Taylor 1989, pp. 401-402). However, if a small amount of Ti is present (<0.05 mol fraction) in the solution, it inhibits hematite formation and favors the formation of goethite (Fitzpatrick et al. 1978).

Other minerals that potentially could form based on the geochemical system at Yucca Mountain are Fe carbonates and Fe-rich silicates. With the addition of carbonate to the system, some $FeCO_3$ [Siderite] would form and is stable in the region shown on Figure 2. A likely iron-rich silicate mineral that may form would be some sort of smectite clay [nontronite] given the low temperature conditions of potential formation.

Iron oxides (and iron-rich clays) have high numbers of surface functional groups and are known to absorb a variety of cations on to their surfaces including U, Np, Pu and Th radionuclides (Viani et al., 1997). Thus, with the potential to have hundreds to thousands of kilograms of iron oxides (Tables 4 and 5) within the repository drift as a result of corrosion progress, adsorption onto Fe corrosion products could significantly retard the release of many of the radionuclides and contain them inside the EBS. In addition to the sorptive capacity of Fe oxides, they tend to incorporate other metallic cations into their crystal structures by isomorphous substitution. Aluminum ions tend to do this the most, however other cations are commonly incorporated into Fe oxides (e.g., Ni, Ti, Mn, Co, Cr, Cu) (Schwertmann and Taylor 1989).

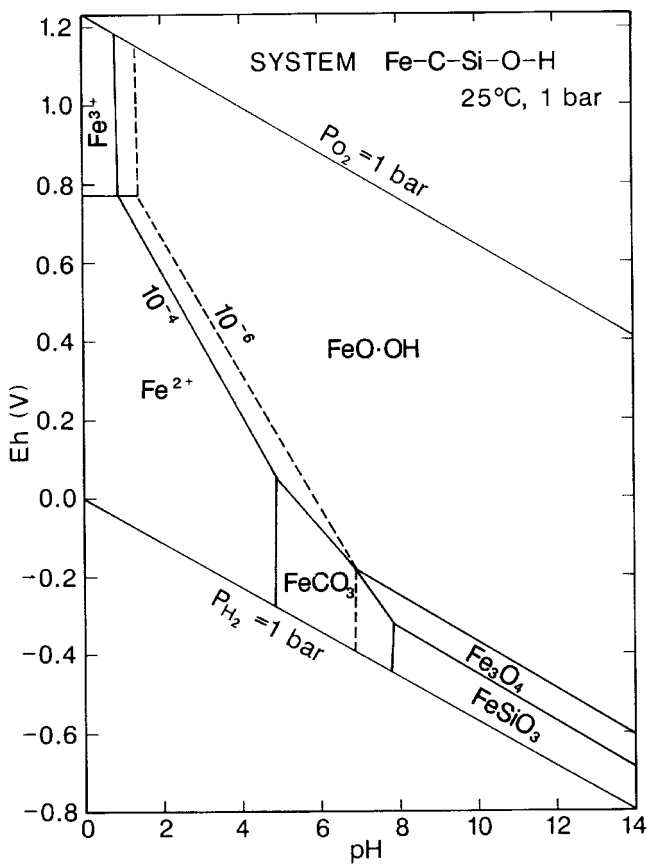

Figure 2. Eh-pH diagram for part of the system Fe-C-Si-O-H. Assumed activities for dissolved species are: Fe = 10-6, Si = 10-3, C = 10-3. Goethite and magnetite assumed as Fe(III) solid phases (Brookins 1988).

Table 7. Typical oxidation-reduction reactions and potential Fe minerals. Designed for Fe minerals using Tebo et al. (1997, Table 2) as an example.

Reaction	Oxidation State	Minerals Formed
$2Fe^{2+} + ½O_2 + 2H_2O = Fe_2O_3 + 4H^+$ $Fe_3O_4 + 2H^+ = Fe_2O_3 + Fe^{2+} + H_2O$ $2FeOOH + 2H^+ + ½O_2 = Fe_2O_3 + Fe^{2+} + 2H_2O$	3	*Hematite* (α-Fe_2O_3)
$Fe^{2+} + ¼O_2 + {}^3/_2H_2O = FeOOH + 2H^+$ $Fe_3O_4 + H^+ + ½O_2 = Fe_2O_3 + FeOOH$	3	*Goethite* (α-FeOOH)
$3Fe^{2+} + ½O_2 + 3H_2O = Fe_3O_4 + 6H^+$	2.67	*Magnitite* (Fe_3O_4)

6.5.1.2 Manganese (Mn)

Tebo et al. (1997) presents a summary of Mn geochemistry, mineralogy and abiotic oxidation. The following paragraphs present highlights of that summary.

Manganese exists in a number of oxidation states among which the II, III, and IV states are those of the greatest environmental importance. Mn(II) is the soluble form and is stable in the pH 6 to 9 range of natural waters (Table 8). Mn(III) is thermodynamically unstable and does not occur in

the soluble form unless it is in the presence of strong complexing agents such as humic or other organic acids. Mn (III) and Mn(IV) primarily form insoluble oxides and oxyhydroxides (e.g. MnO_2 solubility product is 10^{-41}).

The concentration of dissolved Mn in groundwater is generally controlled by the redox reactions between Mn(II) and Mn(III, IV) and governed by pH (Figure 3). These reactions are thermodynamically favorable but will proceed at a slow rate in the absence of microbes. It is only under more extreme conditions (pH > 8.5 and pO_2 ~ 1 atm) that Mn will oxidize in a few weeks to months. The reaction is often autocatalytic but can be driven by Fe oxides and silicates. Oxidation begins with the precipitation of Mn(III)-bearing oxides [Mn_3O_4] or oxyhydroxides, [MnOOH] which subsequently disproportionate slowly in a second step to form Mn (IV) oxides [MnO_2]. In the environment, Mn oxides are the strongest oxidizing agent encountered other than oxygen. At a pH of 7 they are considerably more oxidizing than Fe oxides, They promote the oxidation of As(III), Co(II), Cr(III) and Pu(III). With the presence of carbonate, Mn may form $MnCO_3$ [rhodochrosite]. Additionally, with the presence of large amounts of iron in the drift environment and if the conditions are favorable for carbonate mineral formation, it would be possible for Fe^{2+} to substitute for Mn^{2+} and form some sort of a solid solution between rodochrosite and siderite (Klein and Hurlbut 1977, p. 333).

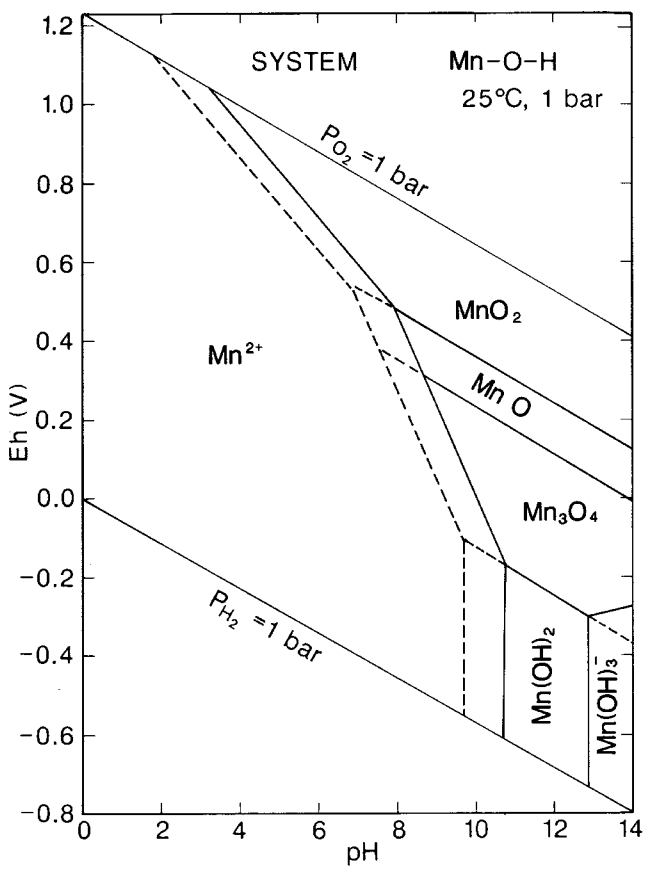

Figure 3. Eh-pH diagram for part of the system Mn-O-H. Assumed activity for Mn = 10^{-6} (Brookins 1988).

Mn oxides are known to absorb a variety of cations on to their surfaces and incorporate other metals in their crystal structure such as Cu, Co, Cd, Zn, and radionuclides such as ^{210}Pb, ^{60}Co, and Ra and Th isotopes. The scavenging of several trace elements by Mn oxides can be so efficient that it results in reduction in the concentration of soluble trace metals by several orders of magnitude.

Table 8. Typical oxidation reactions and potential Mn minerals (modified from Tebo et al, 1997).

Reaction	Oxidation State	Minerals Formed
$Mn^{2+} + ½O_2 + H_2O = MnO_2 + 2H^+$ $Mn_3O_4 + 4H^+ = MnO_2 + 2\ Mn^{2+} + 2H_2O$ $2MnOOH + 2H^+ = MnO_2 + Mn^{2+} + 2H_2O$	4	*Pyrolusite* (β-MnO_2) *Vernadite* (δ-MnO_2)
$Mn^{2+} + ¼O_2 + {}^3/_2H_2O = MnOOH + 2H^+$ $Mn_3O_4 + 2H^+ = 2MnOOH + Mn^{2+}$	3	*Manganite* (γ-MnOOH)
$3Mn^{2+} + ½O_2 + 3H_2O = Mn_3O_4 + 6H^+$	2.67	*Hausmannite* (Mn_3O_4)

6.5.1.3 Nickel (Ni)

Only Ni(II) occurs at ambient environmental conditions. The higher oxidation states occur rarely, and it is not clear whether it is the metal atom rather than the ligand that is oxidized (Cotton and Wilkenson, 1988, p. 741).

There is a general behavior similarity between aqueous Ni and Fe. However, there are some differences. Under oxidizing conditions, nickel hydroxides [$Ni(OH)_2$] are stable at higher pH (between 8 and 12, see Figure 4). Otherwise, either the Ni^{2+} ion or the $HNiO_2^-$ ions are in solution, indicating that nickel is relatively soluble under acidic conditions and under relatively high alkaline conditions (Garrels and Christ 1965).

Nickel tends to substitute for iron and manganese and tends to be co-precipitated as $Ni(OH)_2$ with both iron oxides and manganese oxides (Hem 1985; Hem et al. 1989). Nickel will also adsorb to clays, iron and manganese oxides, and organic matter (McLean and Bledsoe 1992).

6.5.1.4 Chromium (Cr)

Unless otherwise indicated below, the source of most of the summary below was taken from Palmer and Puls (1994).

Chromium exists in oxidation states ranging from +6 to -2, however only the +6 and the +3 oxidation states are commonly encountered in the environment. Cr(VI) exists in solution as monomeric ions $H_2CrO_4^o$, $HCrO_4^-$ (bichromate), and CrO_4^{2-} (chromate), or as the dimeric ion $Cr_2O_7^{2-}$ (bichromate). The relative concentration of each of these species depends on both the pH of the chrome laden water and the total concentration of Cr(VI).

Significant concentrations of $H_2CrO_4^o$ only occur at pH $\leq$ 1. Above pH of 6.5, CrO_4^{2-} generally dominates. Below pH 6.5, $HCrO_4^-$ dominates when the Cr(VI) concentrations are low (<30mM), but $Cr_2O_7^{2-}$ becomes significant when concentrations are greater than 1mM, or it may even dominate when the total Cr(VI) concentrations are greater than 30mM.

In the Cr(III)-H_20 system, Cr(III) exists predominantly as Cr^{3+} below a pH of 3.5. With increasing pH, hydrolysis of Cr^{3+} yields $CrOH^{2+}$, $Cr(OH)_2^+$, $Cr(OH)_3^o$, and $Cr(OH)_4^-$. Under slightly acidic to alkaline conditions, Cr(III) can precipitate as an amorphous chromium hydroxide. Amorphous $Cr(OH)_3$ can crystallize as $Cr(OH)_3 \bullet 3H_2O$ or Cr_2O_3 [eskolaite]. In the presence of Fe(III), trivalent chromium can precipitate as a solid solution. If the pH of the system is between 5 and 12, the aqueous concentration of Cr(III) should be less than 1 µmole/l. In low temperature soil environments that have been contaminated with chromate-laden solutions, $KFe_3(CrO_4)_2(OH)_6$ has been shown to precipitate and can reduce the amount of Cr(VI) in groundwater (Baron and Palmer 1996). This mineral, analogous to the sulfate mineral jarosite, is stable in oxidizing environments between a pH of 2 and 6.

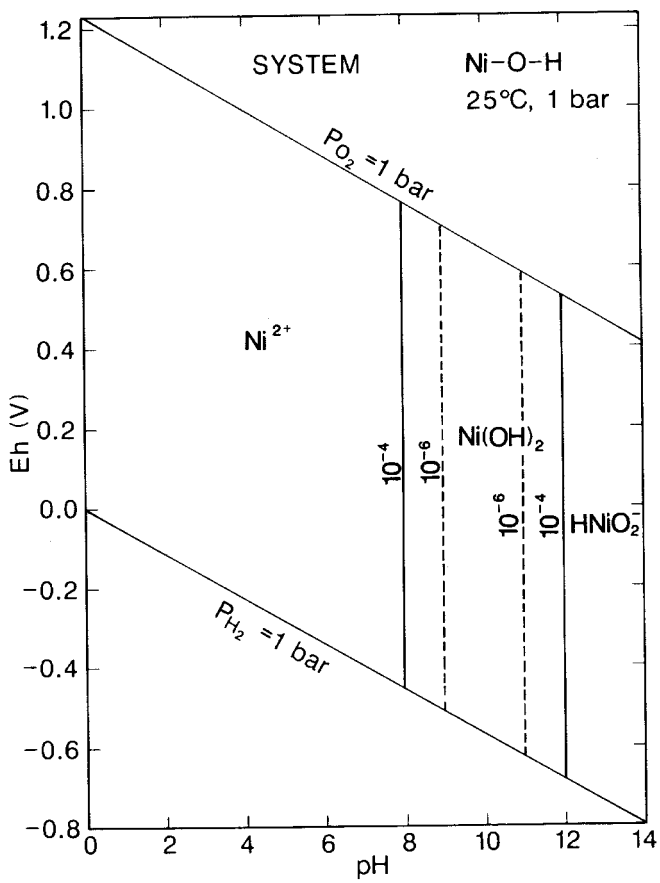

Figure 4. Eh-pH diagram for part of the system Ni-O-H. Assumed activity for Ni = $10^{-4,-6}$ (Brookins 1988).

Cr(VI) is a strong oxidant and is reduced in the presence of electron donors. A common electron donor that could be present in the repository is ferrous iron minerals. This reaction is very fast on the time scales of interest for most environmental problems with the reaction going to completion in about 5 minutes even in the presence of dissolved oxygen (Eary and Rai 1988). When the pH is greater than 10, the rate of oxidation for Fe^{2+} by dissolved oxygen will exceed the rate of oxidation by Cr(VI) (Eary and Rai 1988). When the pH of the groundwater is greater than 4, Cr(III) precipitates with the Fe(III) in a solid solution with the general composition $Cr_xFe_{1-x(}OH)_3$ (Sass and Rai 1987; Amonette and Rai 1990). Therefore, if the pH is between 5 and 12 the concentration of Cr(III) is expected to be less than 10^{-6} molar.

Cr(VI) reduction in the presence of iron oxides, iron-containing silicates, and organic matter has been observed in several experiments. The reduction of Cr(VI) in the presence of hematite (Fe_2O_3) was demonstrated by Eary and Rai (1989). They attribute the reduction to the presence of a small amount of a FeO component in the hematite. They suggest that the reaction occurs in solution after the FeO component has been solubilized. Reduction by biotite occurs when potassium ions are released to solution and Fe^{3+} ions are adsorbed onto the surface of the biotite. Potassium ions are released to maintain charge balance in the biotite structure. Reduction seems to occur even in oxygenated solutions.

Humic and fulvic acids are often associated with reduction by organic matter. The rate of reduction of Cr(VI) by the humic and fulvic acids will decrease with increasing pH. It increases with increasing initial Cr(VI) concentration and increases as the concentration of soil humic substances increases. At neutral pH, complete reduction of Cr(VI) may take many weeks. Sedlak and Chan (1997) studied the reaction of Cr(VI) with Fe(II) with respect to temperature and pH and determined that the reduction of Cr(VI) occurred on the time scale of minutes to months in sediments, soils and waters that contained ferrous iron. Similar type experiments conducted in NaCl, $NaClO_4$, and seawater solutions showed a parabolic dependence on pH, and the influences of temperature, ironic strength, and reductant concentration showed various linearly dependent effects on reduction (Pettine et al. 1998).

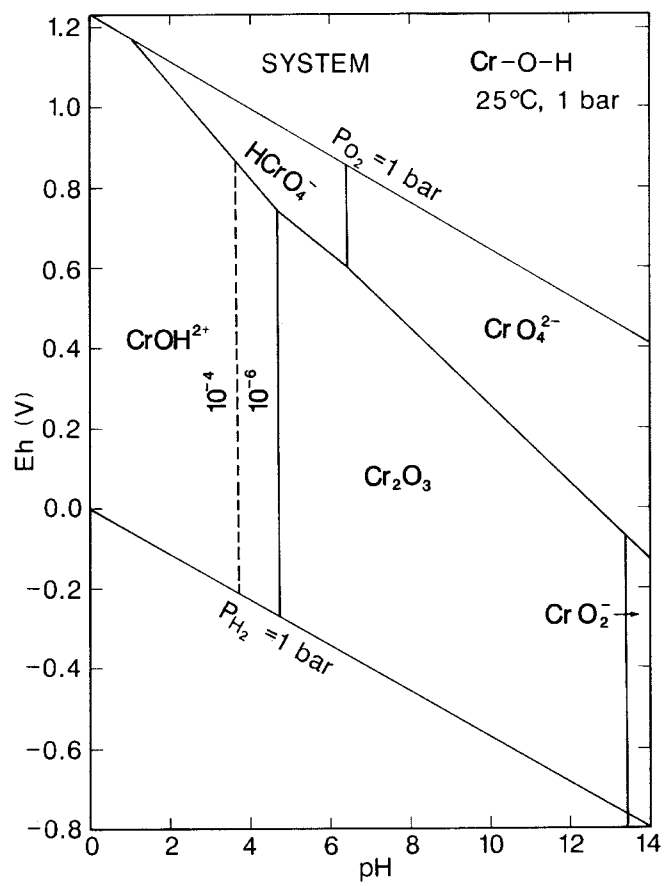

Figure 5. Eh-pH diagram for part of the system Cr-O-H. Assumed activity for Cr = $10^{-4,-6}$ (Brookins 1988).

Oxidation of Cr(III) to CR(VI) can occur in two ways. The first requires dissolved oxygen and the second requires either manganese dioxide (MnO_2) (Eary and Rai 1987) or manganite (MnOOH) (Johnson and Xyla 1991). Eary and Rai (1987) found that dissolved oxygen is not an especially effective nor likely way to oxidize Cr(III). However, interaction with manganese dioxide has been demonstrated to increase as pH decreases and surface area to solution volume increases. Eary and Rai (1987) developed an empirical rate law for the oxidation of Cr(III) by β-MnO_2 [pyrolusite]. For manganite, the rate law has been determined to be independent of pH and ionic strength, however it does proceed slower in the presence of organic ligands (Johnson and Xyla 1991).

Sorption of Cr(VI) onto goethite has been demonstrated to be a surface complexation mechanism dependent on pH. However, on magnetite, the mechanism has been determined to be reductive precipitation onto Fe(II) surface sites (Deng et al. 1996). Competition between common anionic groundwater ions ($CO_{2\ (g)}$, H_4SiO_4, and SO_4^{2-}) and the CrO_4^{2-} ion is known to occur where the adsorption of CrO_4^{2-}onto amorphous iron oxides was suppressed between 50 to 80% (Zachara et al. 1987).

6.5.1.5 Molybdenum (Mo)

In nature, molybdenum occurs in oxidation states ranging from +3 to +6, but the most common solid and aqueous species contain either Mo(IV) or Mo(VI). In oxidizing conditions, the most common state is the +6 state, which forms the following molybdate ions in water: Mo^{6+}, H_2MoO_4, $HMoO_4^-$, and MoO_4^{2-} (Evans et al., 1978). The most prominent species between pH of 2 and 10 is the $HMoO_4^-$ ion and, above pH of 10, the molybdate ion (MoO_4^{2-}) is predominant (Figure 6). Mo has the tendency to enter solution under surface conditions on the earth (Kaback 1976).

Mo solubility controls on concentrations include precipitation in solid solution with common metals. Adsorption, or coprecipitation, of Mo has been documented on a variety of phases: iron and manganese oxides, aluminum oxides and UO_2–MoO_4 oxide complexes (Evans et al. 1978). Adsorption of Mo by amorphous ferric oxyhydroxides has been observed in surface waters and sediments (Kaback and Runnels 1980). Adsorption of Mo on ferric hydroxide is greatest at a pH of 3-4 and decreases with higher or lower pH (Evans et al. 1978). Negatively charged Mo ions also have an affinity for positively charged $Fe(OH)_3$ colloids (Evans et al. 1978). Mo will preferentially sorb to Mn oxides over the Fe oxides. Aluminum oxides will also scavenge Mo at pH values of 4 to 5. In the presence of H_2S at neutral or basic pH, Mo forms soluble thiomolybdates by gradual replacement of oxygen in MoO_4^{2-} (Evans et al. 1978).

6.5.1.6 Titanium (Ti)

The most common and stable oxidation state is Ti(IV) where Ti(IV) compounds are generally covalent (Cotton and Wilkenson 1988, pp. 652-654). Titanium minerals occur mostly in the tetravalent state and are usually octahedrally coordinated with O. Aqueous speciation behavior at 100°C evolves with increasing pH from $Ti(OH)_2^{2+}$ to $TiO_{2(aq)}$ to $Ti(OH)_5^-$ (Knauss et al. 1999). The most common oxide minerals are rutile and ilmenite. However, there are many other silicates and multiple oxide type minerals that form (Milnes and Fitzpatrick 1989, pp. 1132 through 1139).

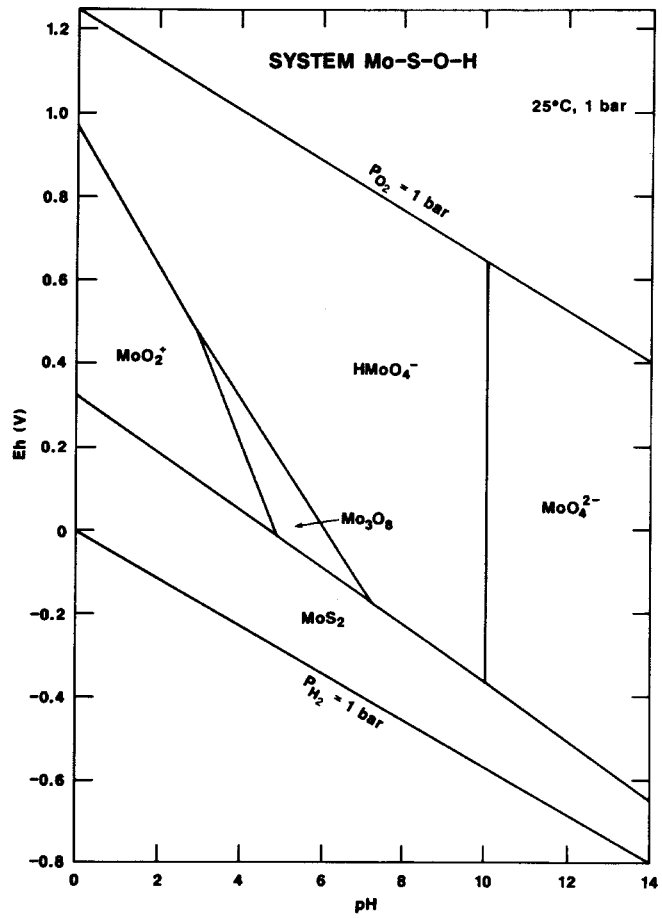

Figure 6. Eh-pH diagram for part of the system Mo-S-O-H. Assumed activity for Mo = 10^{-8},S = 10^{-6} (Brookins 1988).

In soils the common weathering product of titanium minerals seems to be anatase, and the three most common authigenic minerals formed from precipitation reactions are anatase, rutile and ilmanite (Milnes and Fitzpatrick 1989, pp. 1157 through 1162). Rutile is believed to be the stable phase as rutile is thermodynamically stable under ambient conditions (Jamieson and Olinger 1969) and it seems that anatase is a consequence of metastable formation because of sluggish reaction kinetics (Matthews 1976). The dissolution of rutile has been found to be both temperature and pH dependant, with the solubility increasing between temperatures of 100 to 325 °C at both alkaline and acidic pH (Knauss et al. 1999).

From a study of the titanium alloys that could be used for waste package materials, Ti alloys are generally highly corrosion resistant (Gdwoski 1997). Corrosion resistance comes from the formation of very stable insoluble Ti oxide films. Depending on the temperature either anatase or rutile will form from the oxidation of the Ti metal. Gdwoski (1997) described the general sequence at room temperature of the composition of the oxide films on the Ti alloys This seems to follow the sequence shown on Figure 7.

Synthetic solid solutions between Fe and Ti have been precipitated in soils at near ambient conditions (Fitzpatrick et al. 1978). The solid solutions ranged from a mixture of goethite and hematite at low Ti/(Ti+Fe) ratios (≤ 20%; hematite is inhibited at low Ti concentration [< 5 mole

%]), pseudorutile at intermediate ratios (between 20 and 70 %), and anatase at high ratios (>70%).

Surface adsorption of both cations and anions can occur on Ti minerals by two different mechanisms, either specific or nonspecific adsorption (Milnes and Fitzpatrick 1978, p. 1168).

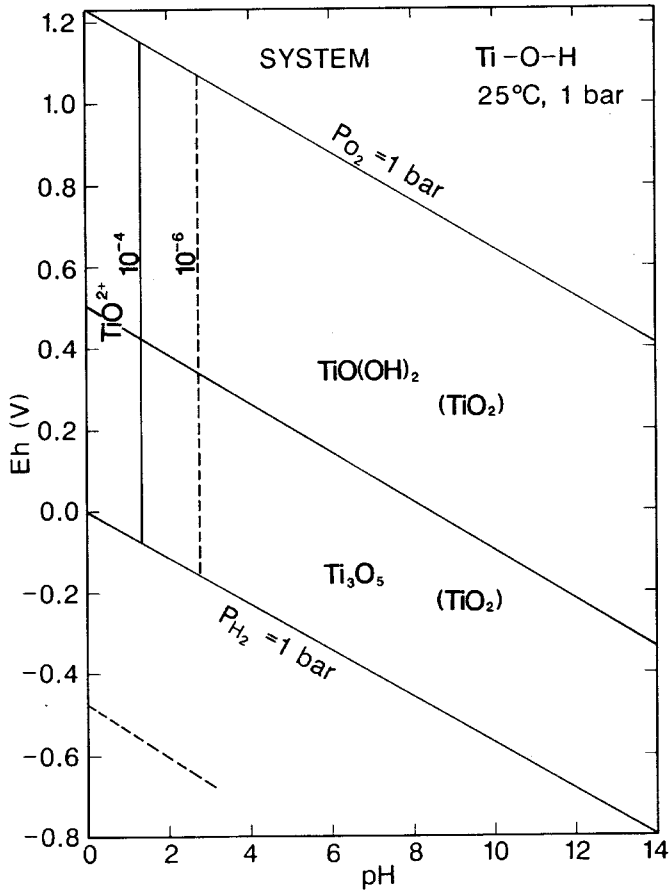

Figure 7. Eh-pH diagram for part of the system Ti-O-H. Assumed activity for Ti = 10^{-6}. Note TiO_2 occupies all Eh-pH space shown as $TiO(OH)_2$ and Ti_30_5 (Brookins 1988).

6.5.1.7 Aluminum (Al)

Al^{3+} predominates in aqueous aluminum solutions where the pH is less than 4, and AlO_2^- predominates above a pH of 11 (See Figure 8). However, at the intermediate pH Al often forms metastable polymeric species with water with a structural pattern of gibbsite (Hsu 1989, p. 347). These polymers eventually form crystalline $Al(OH)_3$.

Three polymorphs of $Al(OH)_3$ exist [bayerite, nordstrandite, and gibbsite] however, in soils only gibbsite is common (Hsu 1989, p. 358). This is attributed to the slow formation of $Al(OH)_3$ in soil environments as opposed to the laboratory experiments from which bayerite and nordstrandite can be rapidly precipitated. Gibbsite, goethite, and hematite are often found in conjunction with each other as the products of advanced weathering of soils (Hsu 1989, p. 358-359).

Aluminum oxyhydroxides [boehmite or diaspore] are also known to form under ambient temperature conditions. The standard free energy change for the $Al(OH)_3$ to AlOOH reaction is close to zero with the value either being positive or negative depending on what free energies of formation are chosen for the calculation (Hsu 1989, p. 362). Hsu (1989) also reports that soils formed in an arid climate would also favor the formation of boehmite and diaspore.

In the presence of sufficient silica, Al is precipitated rapidly to form clay minerals (Hem et al. 1973). $Al(OH)_3$ is known to adsorb both anions and cations. Anions are governed by three types of adsorption mechanisms: nonspecific (positively charged surfaces), specific (chemically adsorbed via ligand exchange), and specific adsorption of anions of incompletely dissociated acids (exchange with OH^-) (Hsu 1989, p. 365). Most polyvalent cations with the exception of Sr and B cations are adsorbed below the point of zero charge (pH 9.4) (Hsu 1989, p. 368).

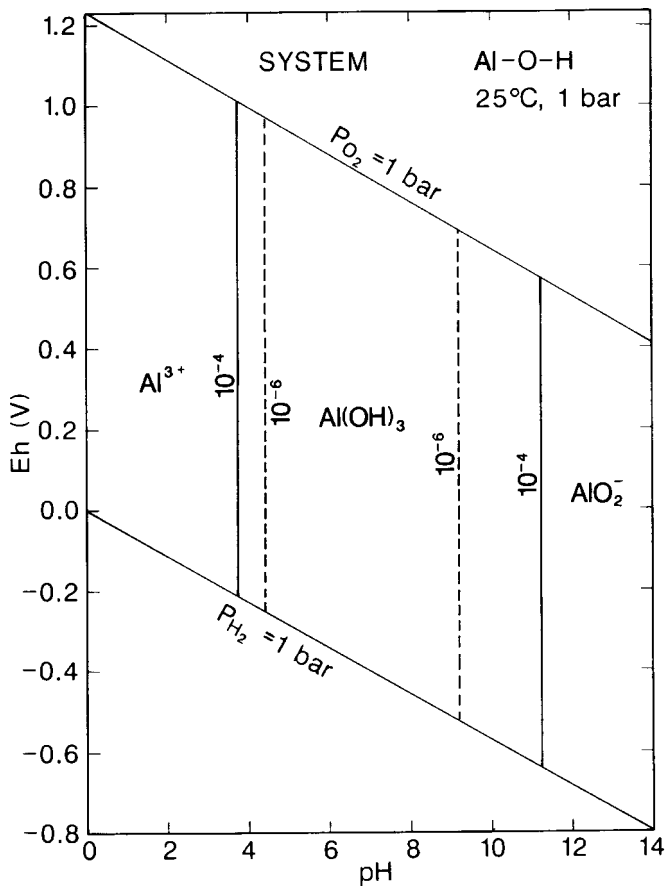

Figure 8. Eh-pH diagram for part of the system Al-O-H. Assumed activity for Al = $10^{-4,-6}$ (Brookins 1988).

6.5.2 Potential Evolution of Metals in the Drift

6.5.2.1 Corrosion Rates

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 in the repository 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).

6.5.2.2 Corrosion Products

Under low oxygen conditions that could be present during the high drift temperatures after waste emplacement, the rate of steel corrosion could dominate the reactions involving free oxygen and drive the drift into a reducing environment. Other possibilities include the rate at which corrosion products become available for radionuclide sorption and whether other dissolved metal species would compete with the radionuclides for sorption sites. This competition would then control the establishment of appropriate sorption coefficients (Kd's) for EBS transport calculations.

The discussions above of each of the elements that make up the steel and alloys indicate that there could be several different compositions of corrosion products. With actual quantities of introduced materials depending on the final repository design, there could be significant amounts of iron oxides (hematite or goethite) formed over time in all areas of the repository drift including inside the waste packages. This is due to the large overall abundance of iron in the steel and alloys that are anticipated to be used in the fabrication of the repository components. Solids formed from other elements such as Mn, Cr, Mo, and Ni will be either in the form of a specific metal oxide mineral (MnO_2, $Ni(OH)_2$, Cr_2O_3, Mo_3O_8, TiO_2, or $Al(OH)_3$) or in some form of solid solution oxide or hydroxide, most likely with Fe mineral (e.g. $Cr_xFe_{1-x}(OH)_3$). Additionally, the Fe and Mn oxides could sorb significant amounts of the other metal ions that could be present in the water reacting in the drift. However, these sorption reactions may be greatly controlled by the composition of the solution chemistry, as much of the sorption is pH dependent.

6.5.2.3 Aqueous Species

At moderate to high pH of the fluids found in the repository drift, most of the metals should end up precipitating as solids, with the exception of perhaps the Cr and Mo species. These two elements have relatively high solubilities under oxidizing conditions and will tend to form CrO_4^{2-} and MoO_4^{2-} ions. Under low pH conditions, most of the metals should be rather soluble with the exception of Ti. Titanium is generally always found as a TiO_2 solid at low temperatures. Any aqueous titanium at low pH should be in the form of $Ti(OH)_2^{2+}$ The ions that should dominate are Fe^{2+}, Mn^{2+}, Ni^{2+}, $CrOH_2^+$, $HMoO^-$ and Al^{3+}. Again, at very high pH the metals will tend to be

rather soluble with the exception of Ti, Mn and Fe. Aqueous species that would tend to form are $HNiO^{2-}$, CrO_4^{2-}, MoO_4^{2-}, $Ti(OH)_5$- and AlO_2^-.

6.5.2.4 Colloids

Colloids are being dealt with in a different sub-model document (CRWMS M&O 1999a). However, with the introduced materials expected to be present in the drift, it is possible to have colloids generated by corrosion of the introduced materials. The two elements that significantly could contribute colloids via corrosion processes are Fe and Al. Iron-oxyhydroxide colloids generated from corrosion processes could be a large source when compared to the natural iron-oxyhydroxide colloids flowing in the groundwater going through the drift. Additionally, Al-hydroxide colloids may be formed from the corrosion of the aluminum materials in the waste packages. Al tends to form polymeric species in solution as well as precipitate clay minerals in the presence of silicates. However, the generation of colloids will be dependent on the corrosion rates of the given material. One detrimental impact to EBS performance from the formation of these colloids is the irreversible sorption of radionuclides to the colloids themselves. The sorbed radionuclides can then be readily transported from the EBS.

6.5.2.5 Microbial Activity

Microbial activity is being dealt with in a different sub-model document (CRWMS M&O 1999a). However, the steels and alloys are large potential source of energy for microbial catalysis. This will influence the size and abundance of microbial communities that could potentially grow in the drift. The result of microbial catalysis is the localized generation of various metal oxides or the localized dissolution of the alloys or metal oxides depending on the redox state of the microenvironment in which the microbes reside.

6.5.3 Bounding In-drift Processes Influencing or Being Influenced by Corrosion Products

With the potential eventual breakdown of the EBS and the waste packages, radionuclides will be available for transport from the repository drift. The solubility of the radionuclides will be established by the aqueous geochemistry in the drift. This geochemistry will be controlled by the quantities of water, gases, and introduced materials that are found within the drift and their overall interaction with the waters fluxing through the EBS, the waste packages, and the waste forms.

Not only do the mobilization and transport of the waste form depend on the rate of corrosion at which the waste package is penetrated, they also depend on (a) the accumulation of corrosion products through which the dissolved radionuclides must travel, (b) the geochemical composition of the water in contact with the waste, (c) the redox state of the in-drift chemical environment, and (d) the evolution of the porosity and permeability of the in-drift environment. A major component of the in-drift environment will be the evolution of the steels and alloys into corrosion products.

6.5.3.1 Waste Form Mobilization

One of the essential parameters that will influence the dissolution of the waste form is pH. Studies have been performed on the pH dependence of the dissolution of spent fuel and DHLW glass. These types of studies have been incorporated into the TSPA calculations in the past (CRWMS M&O 1998c, CRWMS M&O 1995) where the solubility of DHLW glass and CSNF are dependent on pH. Previous geochemical calculations have assumed that Cr and to a lesser extent Mo have the potential to reduce pH in aqueous solutions coming in contact with the waste form (CRWMS M&O 1998g; CRWMS M&O 1998h). This is the result of the oxidation of Cr and Mo to the chromate (or dichromate) and molybdate ion respectively. The principal source in the EBS environment for chromium is in the steel and alloys that are being used in waste package materials.

Again, competing factors between having either potentially slow or fast corrosion rates might play against each other for improved EBS performance. There may be times when the environment is oxygen-limited due to the effects of having elevated temperatures during the high thermal pulse. A slow corrosion rate of steel and alloys results in a lower level of oxygen consumption in the corrosion process. This would allow more oxygen to interact with the reduced waste form and would facilitate the release of technetium and iodine species that are mobile in oxidizing conditions. A rapid corrosion rate would consume greater amounts of oxygen and would allow the waste form to stay in its current configuration longer. However, this would only continue as long as the oxygen availability was depleted and reducing conditions dominated. Once the $O_{2(gas)}$ availability is sufficiently high, the benefits of a reducing environment would disappear.

6.5.3.2 EBS Transport

One of the chief impacts that will occur due to the corrosion of the waste package and degradation of the EBS is the alteration of the transport characteristics of the "as built" repository. The corrosion rate of each introduced material will essentially contribute to both the pathway and the geochemical environment from which any radionuclide in solution may be transported. The inverts and steel sets are generally constructed of carbon steel, which is very susceptible to corrosion and will most likely fail first. However, as these EBS materials fail they will change the porosity and permeability of the in-drift environment.

Obvious potential changes in permeability could come from the accumulation of corrosion materials beneath the waste package. Due to oxidation of steel and alloys, there could be a significant volume expansion; thus, potential plugging of transport pathways through the invert or drift wall may occur. With waste package corrosion (whether corrosion occurs rapidly or slowly) there will be pathways for water flow into and out of the waste package, thus allowing the dissolution of the waste form itself. These pathways essentially may be lined with corrosion products and not with fresh alloy or steel.

Finally, the presence of large amounts of iron oxides and other metal oxides in the transport pathway could significantly retard the release of radionuclides from the repository drifts. As water fluxes through the waste packages and through the corrosion products that are a result of the degradation of the waste package and/or EBS components, both specific and non-specific

sorption mechanisms would be at work, especially those that are associated with iron and manganese oxides.

Conceptually, two competing factors will play against each other for improved EBS performance. A slow corrosion rate of waste package material favors containment within the waste package. However, a fast corrosion rate favors the production of iron or manganese oxides that could act to sorb the radionuclides that would be released form the failed waste packages. However, this would only last as long as there were sorption sites available. Once the sorption sites are exhausted, the benefits of sorption disappear as the attenuation mechanism will be exhausted. Potential sorption of radionuclides may be lessened with the competition for sorption sites by other metal species that are or could be in solution.

7. CONCLUSIONS

7.1 CONCEPTUAL MODEL SUMMARY

Based on the information above, the following are summary statements regarding the evolution of each of the seven elements selected (Fe, Mn, Cr, Ni, Mo, Ti and Al) in the steels and alloys as they form corrosion products.

For iron, the corrosion of the steel and alloys could cause the precipitation of either hematite or goethite depending on pH, temperature and Ti concentration. In the presence of other metals, the hematite or goethite should co-precipitate with those metal ions to form a solid solution. Iron oxides will also act as sorbers for other metals in solution.

For manganese, the corrosion of the steel and alloys could cause the precipitation of pyrolucite. In the presence of iron, Mn could precipitate with hematite or goethite to form a solid solution. Manganese oxides will also act as strong sorbers for other metals in solution.

For nickel, the corrosion of the steel and alloys could cause the precipitation of $Ni(OH)_2$. In the presence of Fe and Mn, Ni could also precipitate with hematite, goethite, or pyrolucite (MnO_2) to form a solid solution. Aqueous nickel tends to sorb onto iron and manganese oxides and will compete with other aqueous metal species for available sorption sites.

For chromium, the corrosion of the steel and alloys could cause the precipitation of Cr_2O_3 especially in the presence of Fe(II). In the presence of Fe(III), Cr could also precipitate with hematite or goethite to form a solid solution. Cr might also be found in solution as CrO_4^{2-}. Aqueous chromium tends to sorb onto iron and manganese oxides and will compete with other aqueous metal species for available sorption sites.

For molybdenum, the corrosion of the steel and alloys may cause the precipitation of Mo_3O_8. However, it is more likely that Mo will be found in solution as MoO_4^{2-}, will precipitate with hematite or goethite to form a solid solution, or will compete with other aqueous metal species for available sorption sites on Fe and Mn oxides.

For titanium, the corrosion of the steel and alloys will cause the precipitation of TiO_2. Ti could also precipitate with hematite or goethite to form a solid solution or it could compete with other aqueous metal species for available sorption sites on Fe and Mn oxides.

For aluminum, the corrosion of the aluminum alloy may cause the precipitation of $Al(OH)_3$ or AlOOH. Al could also precipitate with hematite or goethite to form a solid solution or precipitate as a clay mineral in the presence of silica. Al solids will act as sorbents for both anions and cations in solution.

The above information leads to the following conclusion. Steels and alloys introduced into the repository drift from ground support materials and waste packages will corrode over time. Thus, the aqueous concentrations of metals in the drift will depend on one or more of the following processes:

- Precipitation as a metal oxide or oxyhydroxide.
- Precipitation in a solid solution.
- Acting as either a sorber or sorbent.

A quantitative evaluation of the processes listed above will depend on the availability of metals that could potentially go into aqueous solution. Because the aqueous availability of the above metals will depend on the corrosion rates of each of these materials, the accumulation of corrosion products should ultimately be correlated with the corrosion rates of these materials.

7.2 EXPECTED IMPACT ON IN-DRIFT CHEMICAL ENVIRONMENT

Based on the summary above, only minor impacts are expected to occur in the bulk in-drift chemical environment, with the impacts occurring during active corrosion of the metals and alloys in an oxidizing environment. The largest impact to the aqueous environment should be a decrease in pH due to the oxidation of Cr and Mo to the chromate (or dicromate) and molybdate ion respectively. After formation, corrosion products are generally insoluble in an oxidizing environment and should not affect the composition of the solution further. However, there is a large potential for sorption, which has not been fully quantified nor have its impacts on the bulk in-drift geochemistry been evaluated.

7.3 EVALUATION OF NRC ISSUE RESOLUTION STATUS REPORT CRITERIA

As this documentation contains only the conceptual discussions of the corrosion products submodel of the PAO EBS Physical and Chemical abstracted model, 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 has not been finalized, data uncertainty has not yet 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 has not been finalized, the criteria are not yet addressed.

For Section 4.2.1.4 (Model Verification Acceptance Criteria), these criteria do not apply to the conceptual portions of the models and will be addressed in future work.

7.4 RECOMMENDATIONS FOR FUTURE WORK

Clearly, the concepts discussed herein are of benefit to current analyses as this document provides some basis for assumptions that must be made in other in-drift modeling efforts. Although major impacts to the bulk in-drift geochemical environment are not foreseen, further work is justified. There is not a definite understanding on what impact active corrosion and aqueous chemical composition would have due to a decrease in pH. There also has been limited work done on the impacts of sorption on the bulk geochemistry of the in-drift environment.

Further work should consist of a) modeling the potential changes in pH due to active corrosion; b) quantification of the expected aqueous and solid species; c) quantification of potential corrosion products available for sorption; d) determination of whether competitive sorption onto those corrosion products greatly impacts the radionuclide composition of the water fluxing through the EBS and e) validation of the constructed model.

In order to avoid procedural ambiguity in AP-3.10Q with respect to model validation, this conceptual model has not undergone validation. When one looks at the definitions of model and conceptual model as defined in the procedure, validation would only apply to complete models and not to conceptual models.

7.5 TO BE VERIFIED (TBV) IMPACT

There should be no significant impact to this conceptual model due to the use of the TBV inputs used in constructing Tables 1 and 2. The tables were used to confirm that the seven elements (Fe, Mn, Ni, Mo, Cr, Ti and Al) discussed in this document individually were indeed greater than 1% of the total composition of introduced materials.

7.6 FEP'S EVALUATION

Although the issues found in Table 3 are discussed in this conceptual model, the issues cannot be fully resolved until this conceptual model is utilized in further modeling work.

8. INPUTS AND REFERENCES

8.1 DOCUMENTS CITED

Amonette, J.E. and Rai, D. 1990. "Identification of Noncrystalline (Fe,Cr)(OH)3 by Infrared Spectroscopy." *Clays and Clay Minerals, 38* (2), 129-136. Boulder, Colorado: Clay Minerals Society. TIC: 243615.

Arthur, R.C. and Murphy, W.M. 1989. "An Analysis of Gas-Water-Rock Interactions During Boiling in Partially Saturated Tuff." *Science Geology Bulletin, 42* (4), 313-327. Strasbourg, France: Sciences Geologiques Bulletin Publisher Strasbourg, Universite Louis Pasteur de Strasbourg, Institue. TIC: 235013.

Baron, D. and Palmer, C.D. 1996. "Solubility of KFe3(CrO4)2(OH)6 at 4 to 35[degrees]C." *Geochimica et Cosmochimica Acta, 60* (20), 3815-3824. New York, New York: Elsevier Science. TIC: 243731.

Benson, L.V.; Robison, J.H.; Blankennagel, R.K.; and Ogard, A.E. 1983. *Chemical Composition of Ground Water and the Locations of Permeable Zones in the Yucca Mountain Area, Nevada.* Open-File Report 83-854. Denver, Colorado: U.S. Geological Survey. ACC: NNA.19870610.0028.

Brookins, D.G. 1988. *Eh-pH Diagrams for Geochemistry.* Berlin, Germany: Springer-Verlag. TIC: 237943.

Codell, R.B. and Murphy, W.M. 1992. "Geochemical Model for 14C Transport in Unsaturated Rock." *Proceedings of the Third International Conference on High Level Radioactive Waste Management, Las Vegas, Nevada, April 12-16, 1992,* 1959-1965. La Grange Park, Illinois: American Nuclear Society. TIC: 238761.

Cotton, F.A. and Wilkinson, G. 1988. *Advanced Inorganic Chemistry, 5th Edition.* New York, New York: John Wiley and Sons. TIC: 236867.

CRWMS M&O 1995. *Total System Performance Assessment - 1995: An Evaluation of the Potential Yucca Mountain Repository.* B00000000-01717-2200-00136 REV 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19960724.0188.

CRWMS M&O 1997. *UZ Thermohydrology Drift-Scale Analyses, Provide Input to XPA07, PA204, PA208, PA210 Models.* TR543FB3. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980205.0251.

CRWMS M&O 1998a. "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 1998b. "Geochemistry." Book 3 - Section 6,7 *Yucca Mountain Site Description.* B00000000-01717-5700-00019 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980729.0052.

CRWMS M&O 1998c. "Waste Form Degradation, Radionuclide Mobilization, and Transport Through the Engineered Barrier System." Chapter 6 of *Total System Performance Assessment-Viability Assessment (TSPA-VA) Analyses Technical Basis Document.* B00000000-01717-4301-00006 REV 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19981008.0006.

CRWMS M&O 1998d. "Thermal Hydrology." Chapter 3 of *Total System Performance Assessment-Viability Assessment (TSPA-VA) Analyses Technical Basis Document.* B00000000-01717-4301-00003 REV 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19981008.0003.

CRWMS M&O 1998e. "Geology." Book 1 - Section 3 *Yucca Mountain Site Description.* B00000000-01717-5700-00019 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980729.0049.

CRWMS M&O 1998f. "Hydrologic System." Book 2 - Section 5 *Yucca Mountain Site Description.* B00000000-01717-5700-00019 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980729.0051.

CRWMS M&O 1998g. *EQ6 Calculations for Chemical Degradation of Fast Flux Test Facility (FFTF) Waste Packages.* BBA000000-01717-0210-00028 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19981229.0081.

CRWMS M&O 1998h. *EQ6 Calculations for Chemical Degradation of PWR LEU and PWR MOX Spent Fuel Waste Packages.* BBA000000-01717-0210-00009 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980701.0483.

CRWMS M&O 1999a. *Development Plan (DP) Checklist and Cover Sheet: Provide Sub-Models for the Physical and Chemical Environmental Abstraction Model for TSPA-LA*. 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. *Development Plan (DP) Checklist and Cover Sheet for the 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 1999d. *Request for Repository Subsurface Design Information to Support TSPA-SR.* Input Transmittal PA-SSR-99218.Ta. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990901.0312.

CRWMS M&O 1999e. *Waste Package Design Input for Geochemical Analysis.* Input Transmittal PA-WP-99294.Ta. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19991015.0303.

CRWMS M&O 1999f. *Waste Package Design Input for Geochemical Analysis.* Input Transmittal PA-WP-99294.T. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19991014.0108.

CRWMS M&O 1999g. *Waste Package Materials Properties.* BBA000000-01717-0210-00017 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990407.0172.

CRWMS M&O 1999h. *License Application Design Selection Report.* B00000000-01717-4600-00123 REV 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990528.0303.

CRWMS M&O 1999i. *Yucca Mountain Project (YMP) Features, Events & Processes (FEP) Database.* Revision 00B. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19991025.0084.

Deng, Y.; Stjernstrom, M.; and Banwart S. 1996. "Accumulation and Remobilization of Aqueous Chromium (VI) at Iron Oxide Surfaces: Application of a Thin-film Continuous Flow-through Reactor." *Journal of Contaminant Hydrology, 21*, 141-151. Amsterdam, The Netherlands: Elsevier Science B.V. TIC: 243062.

Eary, L.E. and Rai, D. 1987. "Kinetics of Chromium(III) Oxidation to Chromium(VI) by Reaction with Manganese Dioxide." *Environmental Science and Technology, 21* (12), 1187-1193. Washington, D.C.: American Chemical Society. TIC: 243224.

Eary, L.E. and Rai, D. 1988. "Chromate Removal from Aqueous Wastes by Reduction with Ferrous Ion." *Environmental Science Technology, 22* (8), 972-977. Washington, D.C.: American Chemical Society. TIC: 243600.

Eary, L.E. and Rai, D. 1989. "Kinetics of Chromate Reduction by Ferrous Ions Derived from Hematite and Biotite at 25C." *American Journal of Science, 289*, 180-213. New Haven, Connecticut: Yale University. TIC: 243614.

Evans, H.T.; Manheim, F.T.,Jr.; and Landergren, S. 1978. "Molybdenum 42." *Handbook of Geochemistry: Elements Kr(36) to Ba(56).* Wedepohl, K.H. (ed.). Volume II/4. New York, New York: Springer-Verlag. TIC: 243504.

Fitzpatrick, R.W.; Le Roux, J.; and Schwertmann, U. 1978. "Amorphous and Crystalline Titanium and Iron-Titanium Oxides in Synthetic Preparations, at Near Ambient Conditions, and in Soil Clays." *Clays and Clay Minerals, 26* (3), 189-201. Long Island City, New York: Pergamon. TIC: 242847.

Garrels, R.M. and Christ, C.L. 1965. *Solutions, Minerals and Equilibria.* Boston, Massachusetts: Jones and Bartlett. TIC: 223483.

Gdowski, G.E. 1997. *Degradation Mode Survey Candidate Titanium - Base Alloys for Yucca Mountain Project Waste Package Materials.* UCRL-ID-121191, Rev. 1. Livermore, California: Lawrence Livermore National Laboratory. ACC: MOL.19980120.0053.

Glassley, W. 1997. *Chemical Composition of Water Before Contact with Repository Materials.* Milestone Report SPLA1M4. Livermore, California: Lawrence Livermore National Laboratory. ACC: MOL.19971210.0031.

Glassley, W.E. 1994. *Report on Near-Field Geochemistry: Water Composition Changes Due to Evaporation.* Milestone Report M0L26. Livermore, California: Lawrence Livermore National Laboratory. ACC: MOL.19950406.0153.

Hardin, E.L. 1998. *Near-Field/Altered-Zone Models Report.* UCRL-ID-129179. Livermore, California: Lawrence Livermore National Laboratory. ACC: MOL.19980630.0560.

Harrar, J.E.; Carley, J.F.; Isherwood, W.F.; and Raber, E. 1990. *Report of the Committee to Review the Use of J-13 Well Water in Nevada Nuclear Waste Storage Investigations.* UCID-21867. Livermore, California: Lawrence Livermore National Laboratory. ACC: NNA.19910131.0274.

Hem J. D. 1992. *Study and Interpretation of the Chemical Caracteristics of Natural Water, Third Edition.* U.S. Geological Survey Water Supply Paper 2254. Washington, D.C.: U.S. Geological Survey. TIC: 243429.

Hem, J.D.; Lind, C.J.; and Roberson, C.E. 1989. "Coprecipitation and Redox Reactions of Manganese Oxides with Copper and Nickel." *Geochimica et Cosmochimica Acta, 53*, 2811-2822. New York, New York: Pergamon Press. TIC: 243113.

Hem, J.D.; Robertson, C.E.; Lind, C.J.; and Polzer, W.L. 1973. "Chemical Interactions of Aluminum with Aqueous Silica at 25°C." *Chemistry of Aluminum in Natural Water.* Water Supply Paper 1827-E. Denver, Colorado: U.S. Geological Survey. TIC: 243428.

Hsu, P.H. 1989. "Chapter 7: Aluminum Hydroxides and Oxyhydroxides." *SSSA Book Series 1: Minerals in Soil Environments, Dixon, J.B. and Weed, S.B. (eds.).* Madison, Wisconsin: Soil Science Society of America. TIC: 237222.

Jamieson, J. C. and Olinger, B. 1969. "Pressure-Temperature Studies of Anatase, Brookite, Rutile and TiO2(II):A Discussion." *The American Mineralogist, 54* (9-10), 1477-1481. Washington, D.C.: Mineralogical Society of America. TIC: 243026.

Johnson, C.A. and Xyla, A.G. 1991. "The Oxidation of Chromium(III) to Chromium(VI) on the Surface of Manganite (MnOOH)." *Geochimica et Cosmochimica Acta, 55*, 2861-2866. New York, New York: Elsevier Science. TIC: 243616.

Kaback, D.S. 1976. "Transport of Molybdenum in Mountainous Streams, Colorado." *Geochimica et Cosmochimica Acta, 40* (6), 581-582. New York, New York: Pergamon Press. TIC: 243599.

Kaback, D.S. and Runnels, D.D. 1980. "Geochemistry of Molybdenum in Some Stream Sediments and Waters." *Geochimica et Cosmochimica Acta, 44*, 447-456. New York, New York: Pergamon Press. TIC: 243732.

Kerrisk, J.F. 1987. *Groundwater Chemistry at Yucca Mountain, Nevada, and Vicinity.* LA-10929-MS. Los Alamos, New Mexico: Los Alamos National Laboratory. ACC: NNA.19870507.0017.

Klein, C. and Hurlbut, C.S., Jr. 1985. *Manual of Mineralogy 20th Edition.* New York, New York: John Wiley and Sons. TIC: 242818.

Knauss, K.G.; Dibley, M.J.; and Bourcier, W.L. 1999. *Plutonium Immobilization Project Plutonium Immobilization: Issue Interim Report Summarizing Hafnium and Titanium Data (Milestone 4.2b).* PIP-99-051. Livermore, California: Lawrence Livermore National Laboratory. TIC: 243837.

Krauskopf, K B. 1979. *Introduction to Geochemistry, Second Edition.* New York, New York: McGraw-Hill. TIC: 242816.

Lichtner, P.C. and Seth, M. 1996. "Multiphase-Multicomponent Nonisothermal Reactive Transport in Partially Saturated Porous Media." *Proceedings of the 1996 International Conference on Deep Geological Disposal of Radioactive Waste, Canadian Nuclear Society,* 3-133 to 3-142. Toronto, Ontario, Canada: Canadian Nuclear Society. TIC: 237969.

Lipman, P.W.; Christiansen, R.L.; and O'Connor, J.T 1966. *A Compositionally Zoned Ash-Flow Sheet in Southern Nevada.* Professional Paper 524-F. Washington, D.C.: U.S. Geological Survey. TIC: 219972.

Matthews, A. 1976. "The Crystallization of Anatase and Rutile from Amorphous Titanium Dioxide under Hydrothermal Conditions." *The American Mineralogist, 61* (5-6), 419-424. Washington, D.C.: Mineralogical Society of America. TIC: 243096.

McLean, J.E. and Bledsoe, B.E. 1992. *Behavior of Metals in Soils.* EPA/540/S-92/018. Washington, D.C.: U.S. Environmental Protection Agency. TIC: 243412.

Means, J.L.; Maest, A.S.; and Crerar, D.A. 1983. *The Organic Geochemistry of Deep Ground Waters and Radionuclide Partitioning Experiments under Hydrothermal Conditions.* ONWI-448. Columbus, Ohio: Battelle Memorial Institute, Office of Nuclear Waste Isolation. TIC: 209098.

Meike, A. and Wittwer, C. 1993. "Formation of Colloids from Introduced Materials in the Post-Emplacement Environment: A Report on the State of Understanding." *Proceedings of the Topical Meeting on Site Characterization and Model Validation, Focus '93, September 26-29, 1993, Las Vegas, Nevada,* 95-102. La Grange Park, Illinois: American Nuclear Society. TIC: 238492.

Milnes, A.R. and Fitzpatrick, R.W. 1989. "Titanium and Zirconium Minerals ." *Minerals in Soil Environment.* J.B. Dixon and S.B. Weed eds. 2nd Edition, 1131-1205. Madison, Wisconsin: Soil Science Society of America. TIC: 237222.

Murphy, W.M. 1991. "Performance Assessment Perspectives with Reference to the Proposed Repository at Yucca Mountain, Nevada." *Proceedings from the Technical Workshop on Near-Field Performance Assessment for High-Level Waste Held in Madrid, October 15-17, 1990, P. Sellen, M. Apted, and J. Gago, eds.,* 11-22. Stockholm, Sweden: Swedish Nuclear Fuel and Waste Management Company. TIC: 237757.

Murphy, W.M. 1993. "Geochemical Models for Gas-Water-Rock Interactions in a Proposed Nuclear Waste Repository at Yucca Mountain." *Proceedings of the Topical Meeting on Site Characterization and Model Validation, Focus '93, September 26-29, 1993, Las Vegas, Nevada,* 115-121. La Grange Park, Illinois: American Nuclear Society. TIC: 241436.

Murphy, W.M. and Pabalan, R.T. 1994. *Geochemical Investigations Related to the Yucca Mountain Environment and Potential Nuclear Waste Repository.* NUREG/CR-6288. San Antonio, Texas: Southwest Research Institute. TIC: 227032.

Ogard, A.E. and Kerrisk, J.F. 1984. *Groundwater Chemistry Along Flow Paths Between a Proposed Repository Site and the Accessible Environment.* LA-10188-MS. Los Alamos, New Mexico: Los Alamos National Laboratory. ACC: HQS.19880517.2031.

Palmer, C.D. and Puls, R.W. 1994. *Natural Attenuation of Hexavalent Chromium in Ground Water and Soils.* EPA/540/S-94/505. Washington, D.C.: U.S. Environmental Protection Agency. TIC: 243413.

Pankow, J.F. 1991. *Aquatic Chemistry Concepts.* Chelsea, Michigan: Lewis Publishers. TIC: 242999.

Peters, C.A.; Yang, I.C.; Higgins, J.D.; and Burger, P.A. 1992. "A Preliminary Study of the Chemistry of Pore Water Extracted from Tuff by One-Dimensional Compression." *Proceedings of 7th International Symposium on Water-Rock Interaction, 1, Y. K. Kharaka and A. Maest, eds.,* 741-745. Rotterdam, The Netherlands: A.A. Balkema. TIC: 222013.

Pettine, M.; D'Ottone, L.; Campanella, L.; Millero, F.J.; and Passino, R. 1998. "The Reduction of Chromium(VI) by Iron(II) in Aqueous Solutions." *Geochimica et Cosmoch1mica Acta, 62* (9), 1509-1519. New York, New York: Pergamon Press. TIC: 243059.

Pruess, K.; Wang, J.S.Y.; and Tsang, Y.W. 1990a. "On Thermohydrologic Conditions Near High-Level Nuclear Wastes Emplaced in Partially Saturated Fractured Tuff: 2. Effective Continuum Approximation." *Water Resources Research, 26* (6), 1249-1261. Washington, D.C.: American Geophysical Union. TIC: 224854.

Pruess, K.; Wang, J.S.Y.; and Tsang, Y.W. 1990b. "On Thermohydrologic Conditions Near High-Level Nuclear Wastes Emplaced in Partially Saturated Fractured Tuff: 1. Simulation Studies with Explicit Consideration of Fracture Effects." *Water Resources Research, 26* (6), 1235-1248. Washington, D.C.: American Geophysical Union. TIC: 221923.

Sass, B.R. and Rai, D. 1987. "Solubility of Amorphous Chromium(III)-Iron(III) Hydroxide Solid Solutions." *Inorganic Chemistry, 26* (13), 2228-2232. Easton, Pennsylvania: American Chemical Society. TIC: 243717.

Schwertmann, U. and Taylor, R.M. 1989. "Iron Oxides ." *Minerals in Soil Environment, Second Edition.* Dixon J.B. and Weed S.B. eds. SSSA Book Series: 1. 379-438. Madison, Wisconsin: Soil Science Society of America. TIC: 237222.

Sedlak, D.L. and Chan, P.G. 1997. "Reduction of Hexavalent Chromium by Ferrous Iron." *Geochimica et Cosmochimica Acta, 61* (11), 2185-2192. New York, New York: Pergamon Press. TIC: 243064.

Stumm, W. and Morgan, J.J. 1981. *Aquatic Chemistry – An Introduction Emphasizing Chemical Equilibria in Natural Waters.* New York, New York: John Wiley & Sons. TIC: 208448.

Tebo, B. M.; Ghiorse, W. C.; van Wassbergen, L. G.; Siering, P. L.; and Caspi, R. 1997. "Bacterially Mediated Mineral Formation: Insights Into Manganese(II) Oxidation From Molecular Genetic and Biochemical Studies." *Geomicrobiology: Interactions Between Microbes and Minerals.* J.F Banfield and K.H. Nealson, eds. Reviews in Mineralogy, Volume 35, 225-266. Washington, D.C.: Mineralogical Society of America. TIC: 236757.

Triay, I.; Simmons, A.; Levy, S.; Nelson, S.; Nuttall, H.; Robinson, B.; Steinkampf, W.; and Viani, B. 1995. *Colloid-Facilitated Radionuclide Transport at Yucca Mountain.* LA-12779-MS. Los Alamos, New Mexico: Los Alamos National Laboratory. ACC: NNA.19930628.0067.

Viani, B.E.; Torretto, P.C.; and Matzen, S.L. 1997. *Radionuclide Transport through Engineered Barrier System Alteration Products.* Milestone Report SPL3FM4. Livermore, California: Lawrence Livermore National Laboratory. ACC: MOL.19980115.0871.

Wilder, D.G., ed. 1996. *Volume II: Near-Field and Altered-Zone Environment Report.* UCRL-LR-124998. Livermore, California: Lawrence Livermore National Laboratory. ACC: MOL.19961212.0121; MOL.19961212.0122.

Wolery, T.J. 1992a. *EQ3/6, A Software Package for Geochemical Modeling of Aqueous Systems. Package Overview and Installation Guide, (Version 7.0).* UCRL-MA-110662 PTI. Livermore, California: Lawrence Livermore National Laboratory. TIC: 205087.

Wolery, T.J. 1992b. *EQ3NR, A Computer Program for Geochemical Aqueous Speciation-Solubility Calculations. Theoretical Manual, User's Guide, and Related Documentation, (Version 7.0).* UCRL-MA-110662 PT III. Livermore, California: Lawrence Livermore National Laboratory. TIC: 205154.

Wolery, T.J. and Daveler, S.A. 1992. *EQ6, A Computer Program for Reaction Path Modeling of Aqueous Geochemical Systems. Theoretical Manual, User's Guide, and Related Documentation, (Version 7.0).* UCRL-MA-110662 PT IV. Livermore, California: Lawrence Livermore National Laboratory. TIC: 205002.

Yang, I.C. 1992. "Flow and Transport through Unsaturated Rock – Data from Two Test Holes, Yucca Mountain, Nevada." *High Level Radioactive Waste Management, Proceedings of the Third International Conference, Las Vegas, Nevada, April 12-16, 1992, 1,* 732-737. La Grange Park, Illinois: American Nuclear Society. TIC: 204231.

Yang, I.C.; Davis, G.S.; and Sayre, T.M. 1990. "Comparison of Pore-Water Extraction by Triaxial Compression and High-Speed Centrifugation Methods." *Proceedings of Conference on Minimizing Risk to the Hydrological Environment, American Institute of Hydrology,* 250-259. Dubuque, Iowa: Kendall/Hunt Publishing. TIC: 224435.

Yang, I.C.; Turner, A.K.; Sayre, T.M.; and Montazer, P. 1988. *Triaxial-Compression Extraction of Pore Water from Unsaturated Tuff, Yucca Mountain, Nevada.* Water-Resources Investigations Report 88-4189. Denver, Colorado: U.S. Geological Survey. ACC: NNA.19890309.0161.

Zachara, J.M.; Girvin, D.C.; Schmidt, R.L.; and Resch, C.T. 1987. "Chromate Adsorption on Amorphous Iron Oxyhydroxide in the Presence of Major Groundwater Ions." *Environmental Science & Technology, 21* (6), 589-594. Easton, Pennsylvania: American Chemical Society. TIC: 243613.

8.2 CODES, STANDARDS, REGULATIONS, AND PROCEDURES

AP-2.13Q, Rev. 0, ICN 0. *Technical Product Development Planning.* Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.19990701.0617.

AP-3.10Q, Rev. 1, ICN 0. *Analyses and Models.* Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.19990702.0314.

ASTM C 1174-97. *Standard Practice for Prediction of the Long-Term Behavior of Materials, Including Waste Forms, Used in Engineered Barrier Systems (EBS) for Geological Disposal of High-Level Radioactive Waste.* West Conshohocken, Pennsylvania: American Society for Testing and Materials. Readily Available.

ASTM A 572/A 572M-94C E2. 1994. *Standard Specification for High-Strength Low-Alloy Columbium-Vanadium Structural Steel.* West Conshohocken, Pennsylvania: American Society for Testing and Materials. TIC: 241423.

ASTM A759-85. 1985. *Standard Specification for Carbon Steel Crane Rails.* West Conshohocken, Pennsylvania: American Society for Testing and Materials. Readily Available.

ASTM F 432-95. 1995. *Standard Specifications for Roof and Rock Bolts and Accessories.* Philadelphia, Pennsylvania: American Society for Testing and Materials. TIC: 241007.

DOE (U.S. Department of Energy) 1998. *Quality Assurance Requirements and Description.* DOE/RW-0333P, Rev. 8. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.19980601.0022.

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. Readily Available.

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

8.3 SOURCE DATA

MO9807MWDEQ3/6.000. Chapter 4 TSPA-VA Technical Basis Document Near-Field Geochemical Environment. EQ3/6: Corrosion Products Model. Submittal date: 07/15/1998.

9. ATTACHMENTS

Attachment	Title
I	Document Input Reference System DIRS Report

OFFICE OF CIVILIAN RADIOACTIVE WASTE MANAGEMENT
DOCUMENT INPUT REFERENCE SYSTEM

1. Document Identifier No./Rev.:	Change:	Title:
ANL-EBS-MD-000041 Rev. 00		IN DRIFT CORROSION PRODUCTS

Input Document			4. Input Status	5. Section Used in	6. Input Description	7. TBV/TBD Priority	8. TBVDue To		
2a.	2. Technical Product Input Source Title and Identifier(s) with Version	3. Section					Unqual.	From Uncontrolled Source	Un-Confirmed
1	Amonette, J.E. and Rai, D. 1990. "Identification of Noncrystalline (Fe,Cr)(OH)3 by Infrared Spectroscopy." *Clays and Clay Minerals, 38* (2), 129-136. Boulder, Colorado: Clay Minerals Society. TIC: 243615.	General	N/A - Reference Only	6.5.1.4	Reference to the general composition of Iron/chromium solid solutions	N/A	N/A	N/A	N/A
2	Arthur, R.C. and Murphy, W.M. 1989. "An Analysis of Gas-Water-Rock Interactions During Boiling in Partially Saturated Tuff." *Science Geology Bulletin, 42* (4), 313-327. Strasbourg, France: Sciences Geologiques Bulletin Publisher Strasbourg, Universite Louis Pasteur de Strasbourg, Institue. TIC: 235013.	General	N/A - Reference Only	6.2.3	Reference discussing THC reactions in the repository host rock	N/A	N/A	N/A	N/A
3	ASTM C 1174-97. *Standard Practice for Prediction of the Long-Term Behavior of Materials, Including Waste Forms, Used in Engineered Barrier Systems (EBS) for Geological Disposal of High-Level Radioactive Waste.* West Conshohocken, Pennsylvania: American Society for Testing and Materials. TIC: 246015.	General	N/A - Reference Only	4.3	Reference to ASTM standard which applies to EBS modeling	N/A	N/A	N/A	N/A
4	Benson, L.V.; Robison, J.H.; Blankennagel, R.K.; and Ogard, A.E. 1983. *Chemical Composition of Ground Water and the Locations of Permeable Zones in the Yucca Mountain Area, Nevada.* Open-File Report 83-854. Denver, Colorado: U.S. Geological Survey. ACC: NNA.19870610.0028.	General	N/A - Reference Only	6.2.1.2	General reference for water comostitions in the Yucca Mountain subsurface	N/A	N/A	N/A	N/A
5	Brookins, D.G. 1988. *Eh-pH Diagrams for Geochemistry.* New York, New York: Springer-Verlag. TIC: 237943.	General	N/A - Reference Only	6.5.1	Source for Eh-pH diagrams	N/A	N/A	N/A	N/A
6	Baron, D. and Palmer, C.D. 1996. "Solubility of KFe3(CrO4)2(OH)6 at 4 to 35[degrees]C." *Geochimica et Cosmochimica Acta, 60* (20), 3815-3824. New York, New York: Elsevier Science. TIC: 243731.	General	N/A - Reference Only	6.5.1.4	Reference for a specific Fe/Cr mineral soulubility	N/A	N/A	N/A	N/A
7	Cotton, F.A. and Wilkinson, G. 1988. *Advanced Inorganic Chemistry, Fifth Edition.* New York, New York: John Wiley and Sons. TIC: 236867.	18-A, 18-G-2	N/A - Reference Only	6.5.1.3, 6.5.1.6	Reference for specifics on TI and Ni Chemistry	N/A	N/A	N/A	N/A
	CRWMS M&O 1999. Development Plan (DP)	General	N/A -	1.0, 2.0,	Reference to work	N/A	N/A	N/A	N/A

8	Checklist and Cover Sheet: Provide Sub-Models for the Physical and Chemical Environmental Abstraction Model for TSPA-LA. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990902.0450.		Reference Only	6.5.2	direction for this model and to colloid and microbial activity models				
11	CRWMS M&O 1999. *Development Plan (DP) Checklist and Cover Sheet for the 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.	General	N/A - Reference Only	3.2	Reference to Development of GRIM Software Code	N/A	N/A	N/A	N/A
12	CRWMS M&O 1999. *License Application Design Selection Report.* B00000000-01717-4600-00123 REV 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990528.0303.	5.3.2	N/A - Reference Only	5.0, 6.4	Reference to LA Design Selection EDA II description	N/A	N/A	N/A	N/A
15	CRWMS M&O 1999. *Waste Package Design Input for Geochemical Analysis.* Input Transmittal PA-WP-99294.T. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19991014.0108.	Entire	TBV-3523	4.1, 6.4	Preliminary design input for emplaced materials quantities and compositions. Some of the data may be qualified, however, currently these values need to be either qualified or placed in a controlled source	2	X	N/A	N/A
16	CRWMS M&O 1999. *Waste Package Materials Properties.* BBA000000-01717-0210-00017 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990407.0172.	Entire	N/A - Reference Only	4.1, 6.4	Qualified Waste Package Materials Compositions	N/A	N/A	N/A	N/A
		5.9	TBV-3793	4.1.2, 6.4	COMPOSITON OF WASTE PACKAGE ABSORBER PLATES	2	X	N/A	N/A
18	CRWMS M&O 1998. "Waste Form Degradation, Radionuclide Mobilization, and Transport Through the Engineered Barrier System." Chapter 6 of *Total System Performance Assessment-Viability Assessment (TSPA-VA) Analyses Technical Basis Document.* B00000000-01717-4301-00006 REV 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19981008.0006.	General	N/A - Reference Only	6.5.3.1	Reference to pH dependance of waste form dissolution	N/A	N/A	N/A	N/A
19	CRWMS M&O 1995. *Total System Performance Assessment - 1995: An Evaluation of the Potential Yucca Mountain Repository.* B00000000-01717-2200-00136 REV 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19960724.0188.	General	N/A - Reference Only	6.5.3.1	Reference to pH dependance of waste form dissolution	N/A	N/A	N/A	N/A
20	Deng, Y.; Stjernstrom, M.; and Banwart S. 1996. "Accumulation and Remobilization of Aqueous Chromium (VI) at Iron Oxide Surfaces: Application of a Thin-film Continuous Flow-through Reactor."	General	N/A - Reference Only	6.5.1.4	Reference to discussion on sorption of Cr to Fe(II) sites	N/A	N/A	N/A	N/A

	Journal of Contaminant Hydrology, 21, 141-151. Amsterdam, The Netherlands: Elsevier Science B.V. TIC: 243062.								
21	Eary, L.E. and Rai, D. 1987. "Kinetics of Chromium(III) Oxidation to Chromium(VI) by Reaction with Manganese Dioxide." *Environmental Science and Technology, 21* (12), 1187-1193. Washington, D.C.: American Chemical Society. TIC: 243224.	General	N/A - Reference Only	6.5.1.4	Reference on the oxidation of Cr(III)	N/A	N/A	N/A	N/A
22	Eary, L.E. and Rai, D. 1988. "Chromate Removal from Aqueous Wastes by Reduction with Ferrous Ion." *Environmental Science Technology, 22* (8), 972-977. Washington, D.C.: American Chemical Society. TIC: 243600.	General	N/A - Reference Only	6.5.1.4	Reference to strong rate of reaction for Cr as an oxidant of ferrous iron.	N/A	N/A	N/A	N/A
24	Evans, H.T.; Manheim, F.T.,Jr.; and Landergren, S. 1978. "Molybdenum 42." *Handbook of Geochemistry: Elements Kr(36) to Ba(56).* Wedepohl, K.H. (ed.). Volume II/4. New York, New York: Springer-Verlag. TIC: 243504.	General	N/A - Reference Only	6.5.1.5	Reference for discussion on Mo chemistry	N/A	N/A	N/A	N/A
25	Fitzpatrick, R.W.; Le Roux, J.; and Schwertmann, U. 1978. "Amorphous and Crystalline Titanium and Iron-Titanium Oxides in Synthetic Preparations, at Near Ambient Conditions, and in Soil Clays." *Clays and Clay Minerals, 26* (3), 189-201. Long Island City, New York: Pergamon. TIC: 242847.	General	N/A - Reference Only	6.5.1.1, 6.5.1.6	Reference for interactions between aqueous Ti and Fe	N/A	N/A	N/A	N/A
26	Garrels, R.M. and Christ, C.L. 1965. *Solutions, Minerals and Equilibria.* Boston, Massachusetts: Jones and Bartlett. TIC: 223483.	General	N/A - Reference Only	6.5.1.3	Reference to Ni solubility under acidic conditions and under relatively high alkaline conditions	N/A	N/A	N/A	N/A
27	Gdowski, G.E. 1997. *Degradation Mode Survey Candidate Titanium - Base Alloys for Yucca Mountain Project Waste Package Materials.* UCRL-ID-121191, Rev. 1. Livermore, California: Lawrence Livermore National Laboratory. ACC: MOL.19980120.0053.	General	N/A - Reference Only	6.5.1.6	Reference to the sequence of Ti oxide film development	N/A	N/A	N/A	N/A
28	Glassley, W.E. 1994. *Report on Near-Field Geochemistry: Water Composition Changes Due to Evaporation.* Milestone Report M0L26. Livermore, California: Lawrence Livermore National Laboratory. ACC: MOL.19950406.0153.	General	N/A - Reference Only	6.2.3	Reference discussing THC reactions in the repository host rock	N/A	N/A	N/A	N/A
29	Glassley, W. 1997. *Chemical Composition of Water Before Contact with Repository Materials.* Milestone Report SPLA1M4. Livermore, California: Lawrence Livermore National Laboratory. ACC: MOL.19971210.0031.	General	N/A - Reference Only	6.2.3	Reference discussing THC reactions in the repository host rock	N/A	N/A	N/A	N/A
30	Hardin, E.L. 1998. *Near-Field/Altered-Zone Models Report.* UCRL-ID-129179. Livermore, California: Lawrence Livermore National Laboratory. ACC: MOL.19980630.0560.	General	N/A - Reference Only	6.2.3	Reference discussing THC reactions in the repository host rock	N/A	N/A	N/A	N/A

31	Harrar, J.E.; Carley, J.F.; Isherwood, W.F.; and Raber, E. 1990. *Report of the Committee to Review the Use of J-13 Well Water in Nevada Nuclear Waste Storage Investigations.* UCID-21867. Livermore, California: Lawrence Livermore National Laboratory. ACC: NNA.19910131.0274.	General	N/A - Reference Only	6.2.1.2, 6.2.2	Reference to composition of J-13 well water	N/A	N/A	N/A	N/A
33	Hem, J.D.; Robertson, C.E.; Lind, C.J.; and Polzer, W.L. 1973. "Chemical Interactions of Aluminum with Aqueous Silica at 25°C." *Chemistry of Aluminum in Natural Water.* Water Supply Paper 1827-E. Denver, Colorado: U.S. Geological Survey. TIC: 243428.	General	N/A - Reference Only	6.5.1.7	Reference to formation of clays from presence of Al and Si in aqueous solutions.	N/A	N/A	N/A	N/A
34	Hem, J.D.; Lind, C.J.; and Roberson, C.E. 1989. "Coprecipitation and Redox Reactions of Manganese Oxides with Copper and Nickel." *Geochimica et Cosmochimica Acta, 53*, 2811-2822. New York, New York: Pergamon Press. TIC: 243113.	General	N/A - Reference Only	6.5.1.3	Reference to Ni precipitation as a solid solution.	N/A	N/A	N/A	N/A
35	Hsu, P.H. 1989. "Chapter 7: Aluminum Hydroxides and Oxyhydroxides." *SSSA Book Series 1: Minerals in Soil Environments, Dixon, J.B. and Weed, S.B. (eds.).* Madison, Wisconsin: Soil Science Society of America. TIC: 237222.	p. 347-368	N/A - Reference Only	6.5.1.7	Reference to aquesous Al interactions in soils.	N/A	N/A	N/A	N/A
36	Johnson, C.A. and Xyla, A.G. 1991. "The Oxidation of Chromium(III) to Chromium(VI) on the Surface of Manganite (MnOOH)." *Geochimica et Cosmochimica Acta, 55*, 2861-2866. New York, New York: Elsevier Science. TIC: 243616.	General	N/A - Reference Only	6.5.1.4	Reference to oxidation of Cr(III) by MnOOH.	N/A	N/A	N/A	N/A
37	Jamieson, J. C. and Olinger, B. 1969. "Pressure-Temperature Studies of Anatase, Brookite, Rutile and TiO2(II):A Discussion." *The American Mineralogist, 54* (9-10), 1477-1481. Washington, D.C.: Mineralogical Society of America. TIC: 243026.	General	N/A - Reference Only	6.5.1.6	Reference to Rutile stability at ambient conditions.	N/A	N/A	N/A	N/A
38	Kaback, D.S. 1976. "Transport of Molybdenum in Mountainous Streams, Colorado." *Geochimica et Cosmochimica Acta, 40* (6), 581-582. New York, New York: Pergamon Press. TIC: 243599.	General	N/A - Reference Only	6.5.1.5	Reference to solubility of Mo at ambient conditions	N/A	N/A	N/A	N/A
39	Kaback, D.S. and Runnels, D.D. 1980. "Geochemistry of Molybdenum in Some Stream Sediments and Waters." *Geochimica et Cosmochimica Acta, 44*, 447-456. New York, New York: Pergamon Press. TIC: 243732.	General	N/A - Reference Only	6.5.1.5	Reference to sorption of Mo on ferric oxyhydroxides	N/A	N/A	N/A	N/A
40	Knauss, K.G.; Dibley, M.J.; and Bourcier, W.L. 1999. *Plutonium Immobilization Project Plutonium Immobilization: Issue Interim Report Summarizing Hafnium and Titanium Data (Milestone 4.2b).* PIP-99-051. Livermore, California: Lawrence Livermore National Laboratory. TIC: 243837.	General	N/A - Reference Only	6.5.1.6	Reference to Ti speciation under variable pH	N/A	N/A	N/A	N/A
	Kerrisk, J.F. 1987. *Groundwater Chemistry at Yucca*	General	N/A -	6.2.1.2	General reference for	N/A	N/A	N/A	N/A

42	*Mountain, Nevada, and Vicinity.* LA-10929-MS. Los Alamos, New Mexico: Los Alamos National Laboratory. ACC: NNA.19870507.0017.		Reference Only		water compositions in the Yucca Mountain subsurface				
43	Klein, C. and Hurlbut, C.S., Jr. 1985. *Manual of Mineralogy 20th Edition.* New York, New York: John Wiley and Sons. TIC: 242818.	p. 333	N/A - Reference Only	6.5.1.2	Reference to Mn solid solutions.	N/A	N/A	N/A	N/A
44	Krauskopf, K B. 1979. *Introduction to Geochemistry, Second Edition.* New York, New York: McGraw-Hill. TIC: 242816.	p. 208	N/A - Reference Only	6.5.1.1	Reference to slow reaction rate of Gotheite to hematite.	N/A	N/A	N/A	N/A
45	Lichtner, P.C. and Seth, M. 1996. "Multiphase-Multicomponent Nonisothermal Reactive Transport in Partially Saturated Porous Media." *Proceedings of the 1996 International Conference on Deep Geological Disposal of Radioactive Waste, Canadian Nuclear Society,* 3-133 to 3-142. Toronto, Ontario, Canada: Canadian Nuclear Society. TIC: 237969.	General	N/A - Reference Only	6.2.3	Reference discussing THC reactions in the reporsitory host rock.	N/A	N/A	N/A	N/A
46	Lipman, P.W.; Christiansen, R.L.; and O'Connor, J.T 1966. *A Compositionally Zoned Ash-Flow Sheet in Southern Nevada.* Professional Paper 524-F. Washington, D.C.: U.S. Geological Survey. TIC: 219972.	General	N/A - Reference Only	6.2.2	Reference to iron mineral abundance in YM tuffs	N/A	N/A	N/A	N/A
47	Matthews, A. 1976. "The Crystallization of Anatase and Rutile from Amorphous Titanium Dioxide under Hydrothermal Conditions." *The American Mineralogist, 61* (5-6), 419-424. Washington, D.C.: Mineralogical Society of America. TIC: 243096.	General	N/A - Reference Only	6.5.1.6	Reference to slow reactions kinets of TiO minerals.	N/A	N/A	N/A	N/A
48	Milnes, A.R. and Fitzpatrick, R.W. 1989. "Titanium and Zirconium Minerals ." *Minerals in Soil Environment.* J.B. Dixon and S.B. Weed eds. 2nd Edition, 1131-1205. Madison, Wisconsin: Soil Science Society of America. TIC: 237222.	p. 1157-1162	N/A - Reference Only	6.5.1.6	Reference to TiO minerals that form as weathering products.	N/A	N/A	N/A	N/A
49	Means, J.L.; Maest, A.S.; and Crerar, D.A. 1983. *The Organic Geochemistry of Deep Ground Waters and Radionuclide Partitioning Experiments under Hydrothermal Conditions.* ONWI-448. Columbus, Ohio: Battelle Memorial Institute, Office of Nuclear Waste Isolation. TIC: 209098.	General	N/A - Reference Only	6.2.1.2	General reference for water compositions in the Yucca Mountain subsurface	N/A	N/A	N/A	N/A
50	Meike, A. and Wittwer, C. 1993. "Formation of Colloids from Introduced Materials in the Post-Emplacement Environment: A Report on the State of Understanding." *Proceedings of the Topical Meeting on Site Characterization and Model Validation, Focus '93, September 26-29, 1993, Las Vegas, Nevada,* 95-102. La Grange Park, Illinois: American Nuclear Society. TIC: 238492.	General	N/A - Reference Only	6.2.2	Reference to colloids generated from corrosion products	N/A	N/A	N/A	N/A
	Murphy, W.M. 1991. "Performance Assessment	General	N/A -	6.2.3	Reference discussing	N/A	N/A	N/A	N/A

52	Perspectives with Reference to the Proposed Repository at Yucca Mountain, Nevada." *Proceedings from the Technical Workshop on Near-Field Performance Assessment for High-Level Waste Held in Madrid, October 15-17, 1990, P. Sellen, M. Apted, and J. Gago, eds.*, 11-22. Stockholm, Sweden: Swedish Nuclear Fuel and Waste Management Company. TIC: 237757.		Reference Only		THC reactions in the repository host rock.				
53	Murphy, W.M. and Pabalan, R.T. 1994. *Geochemical Investigations Related to the Yucca Mountain Environment and Potential Nuclear Waste Repository.* NUREG/CR-6288. San Antonio, Texas: Southwest Research Institute. TIC: 227032.	General	N/A - Reference Only	6.2.3	Reference discussing THC reactions in the repository host rock.	N/A	N/A	N/A	N/A
54	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.	General	N/A - Reference Only	1.0, 4.2	Reference to the NRC Criteria for License Appication Review	N/A	N/A	N/A	N/A
55	Ogard, A.E. and Kerrisk, J.F. 1984. *Groundwater Chemistry Along Flow Paths Between a Proposed Repository Site and the Accessible Environment.* LA-10188-MS. Los Alamos, New Mexico: Los Alamos National Laboratory. ACC: HQS.19880517.2031.	General	N/A - Reference Only	6.2.1.2	General reference for water compositions in the Yucca Mountain subsurface	N/A	N/A	N/A	N/A
56	Pankow, J.F. 1991. *Aquatic Chemistry Concepts.* Chelsea, Michigan: Lewis Publishers. TIC: 242999.	p. 231	N/A - Reference Only	6.5.1.1	Reference to pH dependant Fe solubility	N/A	N/A	N/A	N/A
57	Peters, C.A.; Yang, I.C.; Higgins, J.D.; and Burger, P.A. 1992. "A Preliminary Study of the Chemistry of Pore Water Extracted from Tuff by One-Dimensional Compression." *Proceedings of 7th International Symposium on Water-Rock Interaction, 1, Y. K. Kharaka and A. Maest, eds.*, 741-745. Rotterdam, The Netherlands: A.A. Balkema. TIC: 222013.	General	N/A - Reference Only	6.2.1.2	General reference for water compositions in the Yucca Mountain subsurface.	N/A	N/A	N/A	N/A
58	Pettine, M.; D'Ottone, L.; Campanella, L.; Millero, F.J.; and Passino, R. 1998. "The Reduction of Chromium(VI) by Iron(II) in Aqueous Solutions." *Geochimica et Cosmochimica Acta, 62* (9), 1509-1519. New York, New York: Pergamon Press. TIC: 243059.	General	N/A - Reference Only	6.5.1.4	Reference to reaction rates of Cr that are dependant on pH, temperature, ionic strength etc.	N/A	N/A	N/A	N/A
60	Sass, B.R. and Rai, D. 1987. "Solubility of Amorphous Chromium(III)-Iron(III) Hydroxide Solid Solutions." *Inorganic Chemistry, 26* (13), 2228-2232. Easton, Pennsylvania: American Chemical Society. TIC: 243717.	General	N/A - Reference Only	6.5.1.4	Reference to composition of Fe-Cr solid solution	N/A	N/A	N/A	N/A
61	Schwertmann, U. and Taylor, R.M. 1989. "Iron Oxides ." *Minerals in Soil Environment, Second Edition.* Dixon J.B. and Weed S.B. eds. SSSA Book	General	N/A - Reference Only	6.5.1.1	General reference on Iron solubility, speciation and precipitation under	N/A	N/A	N/A	N/A

	Series: 1. 379-438. Madison, Wisconsin: Soil Science Society of America. TIC: 237222.				ambient conditions.				
62	Stumm, W. and Morgan, J.J. 1981. *Aquatic Chemistry – An Introduction Emphasizing Chemical Equilibria in Natural Waters.* New York, New York: John Wiley & Sons. TIC: 208448.	General	N/A - Reference Only	6.5.1.1	Reference on stability of iron oxides	N/A	N/A	N/A	N/A
63	Tebo, B. M.; Ghiorse, W. C.; van Wassbergen, L. G.; Siering, P. L.; and Caspi, R. 1997. "Bacterially Mediated Mineral Formation: Insights Into Manganese(II) Oxidation From Molecular Genetic and Biochemical Studies." *Geomicrobiology: Interactions Between Microbes and Minerals.* J.F Banfield and K.H. Nealson, eds. Reviews in Mineralogy, Volume 35, 225-266. Washington, D.C.: Mineralogical Society of America. TIC: 236757.	General	N/A - Reference Only	6.5.1.1, 6.5.1.2	General reference on low temperature manganese chemistry.	N/A	N/A	N/A	N/A
64	Triay, I.; Simmons, A.; Levy, S.; Nelson, S.; Nuttall, H.; Robinson, B.; Steinkampf, W.; and Viani, B. 1995. *Colloid-Facilitated Radionuclide Transport at Yucca Mountain.* LA-12779-MS. Los Alamos, New Mexico: Los Alamos National Laboratory. ACC: NNA.19930628.0067.	General	N/A - Reference Only	6.2.2	Reference on YM colloid concentrations.	N/A	N/A	N/A	N/A
65	Viani, B.E.; Torretto, P.C.; and Matzen, S.L. 1997. *Radionuclide Transport through Engineered Barrier System Alteration Products.* Milestone Report SPL3FM4. Livermore, California: Lawrence Livermore National Laboratory. ACC: MOL.19980115.0871.	General	N/A - Reference Only	6.5.1.1	Reference on sorption of radionuclides on Fe oxides	N/A	N/A	N/A	N/A
66	Wilder, D.G., ed. 1996. *Volume II: Near-Field and Altered-Zone Environment Report.* UCRL-LR-124998. Livermore, California: Lawrence Livermore National Laboratory. ACC: MOL.19961212.0121; MOL.19961212.0122.	General	N/A - Reference Only	6.2.3	Reference to near-field THC interactions	N/A	N/A	N/A	N/A
67	Wolery, T.J. 1992. *EQ3/6, A Software Package for Geochemical Modeling of Aqueous Systems. Package Overview and Installation Guide, (Version 7.0).* UCRL-MA-110662 PTI. Livermore, California: Lawrence Livermore National Laboratory. TIC: 205087.	General	N/A - Reference Only	3.2	Reference to EQ3/6 software	N/A	N/A	N/A	N/A
68	Wolery, T.J. and Daveler, S.A. 1992. *EQ6, A Computer Program for Reaction Path Modeling of Aqueous Geochemical Systems. Theoretical Manual, User's Guide, and Related Documentation, (Version 7.0).* UCRL-MA-110662 PT IV. Livermore, California: Lawrence Livermore National Laboratory. TIC: 205002.	General	N/A - Reference Only	3.2	Reference to EQ3/6 computer software	N/A	N/A	N/A	N/A
	Yang, I.C.; Turner, A.K.; Sayre, T.M.; and Montazer,	General	N/A -	6.2.1.2	General reference for	N/A	N/A	N/A	N/A

69	P. 1988. *Triaxial-Compression Extraction of Pore Water from Unsaturated Tuff, Yucca Mountain, Nevada.* Water-Resources Investigations Report 88-4189. Denver, Colorado: U.S. Geological Survey. ACC: NNA.19890309.0161.		Reference Only		water and gas compositions in teh Yucca Mountain subsurface				
70	Yang, I.C.; Davis, G.S.; and Sayre, T.M. 1990. "Comparison of Pore-Water Extraction by Triaxial Compression and High-Speed Centrifugation Methods." *Proceedings of Conference on Minimizing Risk to the Hydrological Environment, American Institute of Hydrology,* 250-259. Dubuque, Iowa: Kendall/Hunt Publishing. TIC: 224435.	General	N/A - Reference Only	6.2.1.2	General reference for water and gas compositions in the Yucca Mountain subsurface.	N/A	N/A	N/A	N/A
71	Yang, I.C. 1992. "Flow and Transport through Unsaturated Rock – Data from Two Test Holes, Yucca Mountain, Nevada." *High Level Radioactive Waste Management, Proceedings of the Third International Conference, Las Vegas, Nevada, April 12-16, 1992, 1,* 732-737. La Grange Park, Illinois: American Nuclear Society. TIC: 204231.	General	N/A - Reference Only	6.2.1.2	General reference for water and gas compositions in the Yucca Mountain subsurface.	N/A	N/A	N/A	N/A
72	Zachara, J.M.; Girvin, D.C.; Schmidt, R.L.; and Resch, C.T. 1987. "Chromate Adsorption on Amorphous Iron Oxyhydroxide in the Presence of Major Groundwater Ions." *Environmental Science & Technology, 21* (6), 589-594. Easton, Pennsylvania: American Chemical Society. TIC: 243613.	General	N/A - Reference Only	6.5.1.4	Reference to chromate sorption onto iron oxyhydroxides.	N/A	N/A	N/A	N/A
73	Sedlak, D.L. and Chan, P.G. 1997. "Reduction of Hexavalent Chromium by Ferrous Iron." *Geochimica et Cosmochimica Acta, 61* (11), 2185-2192. New York, New York: Pergamon Press. TIC: 243064.	General	N/A - Reference Only	6.5.1.4	Reference to Cr(VI) reduction reaction rates.	N/A	N/A	N/A	N/A
75	CRWMS M&O 1998. "Hydrologic System." Book 2 - Section 5 *Yucca Mountain Site Description.* B00000000-01717-5700-00019 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980729.0051.	General	N/A - Reference Only	6.2.1, 6.2.2	Reference to background information for geochemistry on the site	N/A	N/A	N/A	N/A
78	CRWMS M&O 1998. *EQ6 Calculations for Chemical Degradation of PWR LEU and PWR MOX Spent Fuel Waste Packages.* BBA000000-01717-0210-00009 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980701.0483.	3	N/A - Reference Only	6.5.3.1	Reference to assumptions used for Cr and Mo in previous WPO geochemical calculations.	N/A	N/A	N/A	N/A
80	AP-2.13Q, Rev. 0, ICN 0. *Technical Product Development Planning.* Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.19990701.0617.	General	N/A - Reference Only	2.0	Reference to YMP QA procedures for planning technical work	N/A	N/A	N/A	N/A
81	AP-3.10Q, Rev. 1, ICN 0. *Analyses and Models.* Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.19990702.0314.	General	N/A - Reference Only	2.0	Reference to YMP QA procedures for development of models and analyses	N/A	N/A	N/A	N/A

82	DOE (U.S. Department of Energy) 1998. *Quality Assurance Requirements and Description.* DOE/RW-0333P, Rev. 8. Washington, D.C.: U.S. Department of Energy, Office of Civilian Radioactive Waste Management. ACC: MOL.19980601.0022.	General	N/A - Reference Only	2.0	Reference to basis for YMP QA procedures	N/A	N/A	N/A	N/A
83	QAP-2-0, Rev. 5. *Conduct of Activities.* Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980826.0209.	General	N/A - Reference Only	2.0	Reference to YMP QA procedure for determining if the QA program is applicable to technical work	N/A	N/A	N/A	N/A
84	MO9807MWDEQ3/6.000. Chapter 4 TSPA-VA Technical Basis Document Near-Field Geochemical Environment. EQ3/6: Corrosion Products Model. Submittal date: 07/15/1998.	Entire	N/A - Reference Only	3.2	Reference to TSPA-VA Corrosion Products Model	N/A	N/A	N/A	N/A
85	CRWMS M&O 1997. *UZ Thermohydrology Drift-Scale Analyses, Provide Input to XPA07, PA204, PA208, PA210 Models.* TR543FB3. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980205.0251.	General	N/A - Reference Only	6.2.3	Reference to TSPA-VA thermal hydrological calculations	N/A	N/A	N/A	N/A
86	CRWMS M&O 1998. "Geochemistry." Book 3 - Section 6,7 *Yucca Mountain Site Description.* B00000000-01717-5700-00019 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980729.0052.	General	N/A - Reference Only	6.2.2	Reference to background information for geochemistry on the site	N/A	N/A	N/A	N/A
88	Codell, R.B. and Murphy, W.M. 1992. "Geochemical Model for 14C Transport in Unsaturated Rock." *Proceedings of the Third International Conference on High Level Radioactive Waste Management, Las Vegas, Nevada, April 12-16, 1992,* 1959-1965. La Grange Park, Illinois: American Nuclear Society. TIC: 238761.	General	N/A - Reference Only	6.2.3	Reference to thermal perturbance will affect the flux and compositon of gas entering the potential emplacement drifts	N/A	N/A	N/A	N/A
89	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.	General	N/A - Reference Only	3.2, 6.1, 6.2	Reference to TSPA-VA NFGE corrosion products model	N/A	N/A	N/A	N/A
90	Eary, L.E. and Rai, D. 1989. "Kinetics of Chromate Reduction by Ferrous Ions Derived from Hematite and Biotite at 25C." *American Journal of Science, 289,* 180-213. New Haven, Connecticut: Yale University. TIC: 243614.	General	N/A - Reference Only	6.5.1.4	Reference to reduction of Cr(VI) in presence of hematite	N/A	N/A	N/A	N/A
92	McLean, J.E. and Bledsoe, B.E. 1992. *Behavior of Metals in Soils.* EPA/540/S-92/018. Washington, D.C.: U.S. Environmental Protection Agency. TIC: 243412.	General	N/A - Reference Only	6.5.1.3	Reference to sorption of Ni to metal oxides, clays and organic matter.	N/A	N/A	N/A	N/A
	Murphy, W.M. 1993. "Geochemical Models for	General	N/A -	6.2.3	Reference discussing	N/A	N/A	N/A	N/A

93	Gas-Water-Rock Interactions in a Proposed Nuclear Waste Repository at Yucca Mountain." *Proceedings of the Topical Meeting on Site Characterization and Model Validation, Focus '93, September 26-29, 1993, Las Vegas, Nevada,* 115-121. La Grange Park, Illinois: American Nuclear Society. TIC: 241436.		Reference Only		THC reactions in the repository host rock.				
94	Palmer, C.D. and Puls, R.W. 1994. *Natural Attenuation of Hexavalent Chromium in Ground Water and Soils.* EPA/540/S-94/505. Washington, D.C.: U.S. Environmental Protection Agency. TIC: 243413.	General	N/A - Reference Only	6.5.1.4	General reference on aqueous Cr chemistry	N/A	N/A	N/A	N/A
95	Pruess, K.; Wang, J.S.Y.; and Tsang, Y.W. 1990. "On Thermohydrologic Conditions Near High-Level Nuclear Wastes Emplaced in Partially Saturated Fractured Tuff: 1. Simulation Studies with Explicit Consideration of Fracture Effects." *Water Resources Research, 26* (6), 1235-1248. Washington, D.C.: American Geophysical Union. TIC: 221923.	General	N/A - Reference Only	6.2.3	Reference discussing THC reactions in the repository host rock.	N/A	N/A	N/A	N/A
96	Pruess, K.; Wang, J.S.Y.; and Tsang, Y.W. 1990. "On Thermohydrologic Conditions Near High-Level Nuclear Wastes Emplaced in Partially Saturated Fractured Tuff: 2. Effective Continuum Approximation." *Water Resources Research, 26* (6), 1249-1261. Washington, D.C.: American Geophysical Union. TIC: 224854.	General	N/A - Reference Only	6.2.3	Reference discussing THC reactions in the repository host rock	N/A	N/A	N/A	N/A
98	Wolery, T.J. 1992. *EQ3NR, A Computer Program for Geochemical Aqueous Speciation-Solubility Calculations. Theoretical Manual, User's Guide, and Related Documentation, (Version 7.0).* UCRL-MA-110662 PT III. Livermore, California: Lawrence Livermore National Laboratory. TIC: 205154.	General	N/A - Reference Only	3.2	Reference to EQ3/6 software	N/A	N/A	N/A	N/A
99	CRWMS M&O 1999. *Waste Package Design Input for Geochemical Analysis.* Input Transmittal PA-WP-99294.Ta. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19991015.0303.	Item 2	N/A - Reference Only	4.1, 5, 6.4	Reference to preliminary design data for weight % if boron in waste package design materials.	N/A	N/A	N/A	N/A
100	CRWMS M&O 1998. *EQ6 Calculations for Chemical Degradation of Fast Flux Test Facility (FFTF) Waste Packages.* BBA000000-01717-0210-00028 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19981229.0081.	3	N/A - Reference Only	6.5.3.1	Reference to assumptions used for Cr and Mo in previous WPO geochemical calculations	N/A	N/A	N/A	N/A
101	CRWMS M&O 1998. "Thermal Hydrology." Chapter 3 of *Total System Performance Assessment-Viability Assessment (TSPA-VA) Analyses Technical Basis Document.* B00000000-01717-4301-00003 REV 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19981008.0003.	General	N/A - Reference Only	6.2.3	Reference to TSPA-VA thermal hydrology values	N/A	N/A	N/A	N/A
	CRWMS M&O 1999. *Request for Repository*	Entire	TBV-	4.1, 5.0,	DESIGN INPUT FOR	2	X	N/A	N/A

102	*Subsurface Design Information to Support TSPA-SR.* Input Transmittal PA-SSR-99218.Ta. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990901.0312.		3763	6.4	EMPLACED MATERIALS, QUANTITIES AND COMPOSITONS				
103	CRWMS M&O 1998. "Geology." Book 1 - Section 3 *Yucca Mountain Site Description.* B00000000-01717-5700-00019 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19980729.0049.	General	N/A - Reference Only	6.2.2	Reference to Geology of site	N/A	N/A	N/A	N/A
104	Hem J. D. 1992. *Study and Interpretation of the Chemical Caracteristics of Natural Water, Third Edition.* U.S. Geological Survey Water Supply Paper 2254. Washington, D.C.: U.S. Geological Survey. TIC: 243429.	General	N/A - Reference Only	6.5.1.3	Reference to Ni precipitiation as a solid solution with both iron oxides and manganese oxides	N/A	N/A	N/A	N/A
105	CRWMS M&O 1999. *Yucca Mountain Project (YMP) Features, Events & Processes (FEP) Database.* Revision 00B. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19991025.0084.	General	N/A - Reference Only	4.2.2	Reference for YMP FEP Database	N/A	N/A	N/A	N/A
107	ASTM A 759-85. *Standard Specification for Carbon Steel Crane Rails.* West Conshohocken, Pennsylvania: American Society for Testing and Materials.	General	N/A - Accepted Data (Fact)	4, 5	Compositon of A759 steel	N/A	N/A	N/A	N/A
108	ASTM F 432-95. 1995. *Standard Specifications for Roof and Rock Bolts and Accessories.* Philadelphia, Pennsylvania: American Society for Testing and Materials. TIC: 241007.	General	N/A - Accepted Data (Fact)	4, 5	Compositon of F432 Rock Bolts	N/A	N/A	N/A	N/A
109	ASTM A 572/A 572M-94C E2. 1994. *Standard Specification for High-Strength Low-Alloy Columbium-Vanadium Structural Steel.* West Conshohocken, Pennsylvania: American Society for Testing and Materials. TIC: 241423.	General	N/A - Accepted Data (Fact)	4, 5	Compositon of A 572 Steel	N/A	N/A	N/A	N/A
110	CRWMS M&O 1999. *Conduct of Performance Assessment. Activity Evaluation.* Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19991028.0092.	Entire	N/A - Reference Only	2.0	Reference to QAP-2-0 Activity evaluation for this model	N/A	N/A	N/A	N/A

Note: The numbers in column 2a are not in sequential order. This is an internal problem with the DIRS system. The following are omitted: 9, 10, 13, 14, 17, 23, 32, 41, 51, 59, 74, 76, 77, 79, 87, 91, 97, and 106.

Note: DIRS does not allow insertion of alpha designators to the references as shown in Section 8.