Model
Error Resolution Document

Complete only applicable items.

QA: QA
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INITIATION

1. Originator:	2. Date:	3. ERD No.
Ernest Hardin	03/11/2008	ANL-EBS-MD-000037 ERD 01

4. Document Identifier:	5. Document Title:
ANL-EBS-MD-000037 REV 04 AD01	IN-PACKAGE CHEMISTRY ABSTRACTION

6. Description of and Justification for Change (Identify applicable CRs and TBVs):

Introduction

This document was created for the resolution of 4 TBV's (8633, 8634, 8635 and 8636) and 2 CR's (11151 and 11786). This document presents the disposition of the TBV's and CR's, identifies changes to the AMR and evaluates impact on the conclusions of the AMR.

1.) TBV-8636:

Background Information Summary: Citation to DIRS# 178871 is incorrectly cited as SNL 2007 instead of SNL 2008.

AMR changes:

1.) Section 6.3.10[a] p. 6-68[a]: revise the citation from SNL 2007 [DIRS 178871] to SNL 2008 [DIRS 178871].

2.) Section 9.1[a] p. 9-8[a]: change reference as follows:

178871 SNL (Sandia National Laboratories) 2008. *Total System Performance Assessment Model/Analysis for the License Application.* MDL-WIS-PA-000005 REV 00. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20080204.0003.

Inputs and/or Software: No changes.

Impact Evaluation/Results: The change to the year is reflected on a corrected final DIRS report for ANL-EBS-MD-000037 REV 04 AD01. There is no impact on the conclusions of the AMR from this editorial change.

CONCURRENCE

	Printed Name	Signature	Date
7. Checker	Susan LeStrange	Susan LeStrange	3/24/08
8. QCS/QA Reviewer	Robert Spencer	Robert Spencer	03/24/08

APPROVAL

9. Originator	Ernest Hardin		3/24/08
10. Responsible Manager	Paul Dixon		3-24-08

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2.) TBV-8633:

Background Information Summary: Citation to SNL 2007 [DIRS 181395] is incorrectly cited as an indirect source, the DIRS# should have been SNL 2007 [DIRS 181165].

AMR changes:

1.) Section 6.6.1[a] p. 6-32[a]: Replace two citations from SNL 2007 [DIRS 181395] to SNL 2007 [DIRS 181165] (including the title of the report) as follows:

This effect is also shown in a sensitivity analysis documented in Appendix C of *Geochemistry Model Validation Report: Material Degradation and Release Model* (SNL 2007 [DIRS 181165]). That model simulates the same processes as the waste form IPC model. In the analysis, water saturation (i.e., percentage of void space filled with water) is varied between 3% and 100%. Because the flow rates and degradation rates are held constant, varying the water saturation is equivalent to varying the ratio of water to reactants. Figure C-1 in that report (SNL 2007 [DIRS 181165], Appendix C) shows that the predicted pH values for the various water saturations are very similar over time but that lower water saturations approach steady-state conditions more quickly.

2.) Section 6.6.1[a] p. 6-33[a]: Replace one citation from SNL 2007 [DIRS 181395] to SNL 2007 [DIRS 181165]:

Sensitivity analyses involving this ratio are not included in this addendum because they are included elsewhere (Appendix C of SNL 2007 [DIRS 181165] and Section 6.6.1 of the parent report).

3.) Section 9.1[a], p. 9-7[a]: Replace the reference from SNL 2007 [DIRS 181395] to SNL 2007 [DIRS 181165] as follows:

181165 SNL (Sandia National Laboratories) 2007. *Geochemistry Model Validation Report: Material Degradation and Release Model.* ANL-EBS-GS-000001 REV 02. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070928.0010.

Inputs and/or Software: Change to DIRS numbers as stated above, but no changes to any information used.

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Impact Evaluation/Results: The correction made to this Indirect source is reflected on a corrected final DIRS report for ANL-EBS-MD-000037 REV 04 AD01. There is no impact on the conclusions of the AMR because the information presented was correct, only the wrong DIRS number was cited.

3.) TBV-8634:

Background Information Summary: Correct incorrect citation to Table in the source [DIRS 179394].

AMR changes:

1.) Table 4-7[a]: Replace with first portion of source with:

SNL 2007 [DIRS 179394] Table 4-2 (this applies to the CSNF (TAD) waste packages).

Inputs and/or Software: No changes.

Impact Evaluation/Results: The correction made is reflected on a corrected final DIRS report for ANL-EBS-MD-000037 REV 04 AD01. There is no impact on the conclusions of the AMR because the information presented was correct, only the Table number was incorrect.

4.) TBV-8635:

Background Information Summary: Correct incorrect citation to the source [DIRS 179567].

AMR changes:

1.) Table 4-7[a]: Replace with second portion of source with:

For 2DHLW and 2MCO waste packages, the materials are unchanged, see Section 4.1.4 of the parent report (DHLW (glass- pour canister): BSC 2005 [DIRS 174225], Table 3-1 and MCO: DOE 2000 [DIRS 150095], Section 4).

2.) Section 9.1[a]: add 2 new references:

174225 BSC (Bechtel SAIC Company) 2005. *DOE and Commercial Waste Package System Description Document.* 000-3YD-DS00-00100-000-006. Las Vegas, Nevada: Bechtel SAIC Company. ACC: ENG.20050620.0002.

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150095 DOE (U.S. Department of Energy) 2000. *N Reactor (U-Metal) Fuel Characteristics for Disposal Criticality Analysis.* DOE/SNF/REP-056, Rev. 0. [Washington, D.C.]: U.S. Department of Energy, Office of Environmental Management. TIC: 247956.

Inputs and/or Software: Change to DIRS numbers as stated above, but no changes to any information used.

Impact Evaluation/Results: The correction made is reflected on a corrected final DIRS report for ANL-EBS-MD-000037 REV 04 AD01. There is no impact on the conclusions of the AMR because the information presented was correct, only the DIRS number was incorrect.

5.) CR: 11151:

Background Information Summary: In ANL-EBS-MD-000037 REV 04 the total carbonate calculation units contains a typographical error which cites the units as atmospheres, the correct units are bars.

AMR changes:

1.) Table 6-22, p. 6-133 and Table 6-25, p. 6-136: replace note under source in both tables as follows: Table 6-22: PCO2 is the partial pressure of CO2 (in bars) and Table 6-25 PO_2 is the partial pressure of O_2 (in bars).

Inputs and/or Software: No changes.

Impact Evaluation/Results: This is a typographical error that only applies to two instances where bars are being used for the *k* value in an equation (Tables 6-22 and 6-25). In other references in the report PCO_2 is correctly described in atmospheres. TSPA-LA actually uses bars in their calculations, so there is no impact on TSPA-LA calculations. Also, bars and atmospheres are almost identical: 1 atm = 1.013 bar, so if atm had been used instead of bars, the impact would have been very small.

6.) CR-11786:

Background Information Summary: Incorrect DIRS for Iceland groundwater composition; [DIRS 168716] to be replaced with [DIRS 179957]:

AMR changes:

1.) Table 4-1[a]: Replace the citation on the third line on page 4-5[a] for the BI Water: Gislason and Eugster (1987 [DIRS 168716], Table 3, Sample SP 01) with Gislason and Eugster (1987 [DIRS 179957], Table 3, Sample SP 01).

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2.) Table 4-4[a]: Replace citation to Gislason and Eugster (1987 [DIRS 168716], Table 3) with Gislason and Eugster (1987 [DIRS 179957], Table 3).

3.) Section 4.1.2[a], p. 4-6[a]
The three basalt water compositions in Tables 4-4[a] and 4-5[a] come from two publications. The Icelandic basalt water comes from an article by Gislason and Eugster (1987 [DIRS 179957]).

4.) Section 9.1[a], p. 9-4[a]: replace reference to [DIRS 168716] with [DIRS 179957] as follows:

179957 Gislason, S.R. and Eugster, H.P. 1987. "Meteoric Water-Basalt Interactions. II: A Field Study in N.E. Iceland." *Geochimica et Cosmochimica Acta, 51,* 2841-2855. [New York, New York]: Pergamon. TIC: 259231.

5.) Appendix A[a]: Replace 3 citations to [DIRS 168716] with [DIRS 179957] as follows:

p. A-3[a]: Replace Bullet 4:
4. Gislason, S.R. and Eugster, H.P. 1987. "Meteoric Water-Basalt Interactions. II: A Field Study in N.E. Iceland." *Geochimica et Cosmochimica Acta, 51,* 2841-2855. [New York, New York]: Pergamon. TIC: 259231. [DIRS 179957].

p. A-7[a]: Replace 2 citations to [DIRS 168716] with [DIRS 179957].

Inputs and/or Software: Change to DIRS numbers as stated above, but no changes to any information used.

Impact Evaluation/Results: The correction made to this Indirect source is reflected on a corrected final DIRS report for ANL-EBS-MD-000037 REV 04 AD01. There is no impact on the conclusions of the AMR because the information presented was correct, only the wrong DIRS number was cited.

7.) In the process of justifying the design information used for TBVs-8634 and 8635, an additional interface was identified and also included in the ERD as follows:

Request for integration information:

Does the addendum to *In-Package Chemistry Abstraction* (SNL 2007 [DIRS 180506]) produce in-package pH and concentrations of NO_3 and Cl that are consistent with the solution used in corrosion tests for borated stainless steel?

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Introduction

Calculations documented in *Geochemistry Model Validation Report: Material Degradation and Release Model* (SNL 2007 [DIRS 181165]) use borated stainless steel corrosion rates obtained from tests documented in MO0706ECTBSSAR.000 [DIRS 181380]. These tests used a solution with a composition based on in-package chemistry calculations reported in the original parent document of *In-Package Chemistry Abstraction* (ANL-EBS-MD-000037 REV 04). The test solutions had a pH of 5.5 and NO_3 and Cl concentrations of 0.0025 and 0.004 molal, respectively. The corresponding NO_3/Cl molar ratio was 0.63.

Inputs and/or Software: No changes.

AMR changes: No changes.

Evaluation/Results: Borated stainless steel is a component of the CSNF waste package. The pH abstraction for the CSNF liquid influx case, documented in the addendum to *In-Package Chemistry Abstraction*, is illustrated in Figure 6-41[a] (SNL 2007 [DIRS 180506]). It shows that the minimum pH value is approximately 5.5 at an ionic strength of 0.04 molal. This minimum decreases to approximately 5 and 4.8 as ionic strength increases to 1 and 3 molal, respectively. Ionic strengths much higher than 3 molal imply that the relative humidity is below the threshold for predicting a meaningful pH (Figure 6-50[a] and Section 6.10.9.1[a], SNL 2007 [DIRS 180506]). On the high end, the maximum pH increases with increasing pCO_2 (negative log of the partial pressure of CO_2). At pCO_2 values of 1.5, 3, and 4, the maximum pH is approximately 7, 8, and 9, respectively. Because pH is sampled uniformly between the minimum and maximum pH values (Figure 6-41[a]), the pH of 5.5 used in the corrosion tests is near the low end of the distribution; however, it is within the expected range. The pH abstraction for the vapor influx case is essentially identical to the liquid influx case (Section 6.10.1.2[a], SNL 2007 [DIRS 180506]).

The concentrations of NO_3 and Cl in the corrosion tests are also within the ranges calculated in the addendum simulations. Although in-package chemistry NO_3 and Cl abstractions were not produced for the TSPA-LA model, NO_3 and Cl concentrations were calculated over time in batch reactor EQ6 simulations. The results of the CSNF simulations are documented in the EQ6 *.6o output files in folders *1milyr\CSNF** and *Accum\ndCSNF** in DTN: SN0702PAIPC1CA.001 [DIRS 180113]. While the NO_3 concentration varies from negligible concentrations up to 0.3 molal in vapor influx simulations (NO_3 is a product of stainless steel corrosion), the Cl concentration remains essentially zero because there is no source of Cl in the cell. For liquid influx simulations, the NO_3 concentrations vary from near zero to 1.0 molal, and the Cl concentrations vary from approximately 6×10^{-5} to 0.03 molal. The higher molalities result from the consumption of water by degradation reactions. Thus, while concentrations of NO_3 and Cl in the corrosion tests are within the ranges of the in-package chemistry simulations, they are on the low ends of the ranges in the liquid influx simulations.

The NO_3/Cl molar ratio in the corrosion tests is also within the ranges in the addendum simulations. In the liquid influx output files, the NO_3/Cl molar ratio varies generally between 0.2 and 2000 (with exceptions on the low

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end noted below). The higher values of this ratio occur because of the production of NO_3 by stainless steel corrosion. NO_3 increasingly inhibits corrosion as the NO_3/Cl molar ratio increases, so using a ratio of 0.63 in the corrosion tests is reasonably conservative. There are two liquid influx compositions that cause simulations to have a NO_3/Cl molar ratio below 0.2. The first is a pore water called P33. P33 represents the pore water sample from ESF-HD-PERM-3/34.8-35.1 (Table 4-2[a], SNL 2007 [DIRS 180506]). The low NO_3/Cl molar ratio (0.05) of this sample is observed only in a small percentage of the samples from Yucca Mountain (Figure 6.6-18 and Table 6.6-3, SNL 2007 [DIRS 177412]). More importantly, the low ratio is likely an artifact of insufficient sample preservation prior to analysis (Section 6.6.3, SNL 2007 [DIRS 177412]). Thus, this low ratio is not likely to be representative of in situ pore water. The other simulated liquid influx compositions with a low NO_3/Cl molar ratio are basalt waters. However, the basalt water simulations are only relevant in the igneous intrusion scenario. This evaluation was completed to solely answer the question: "Does the addendum ANL-EBS-MD-000037 REV 04 AD01in-package pH and concentrations of NO_3 and Cl that are consistent with the solution used in corrosion tests for borated stainless steel?" There are no changes to the text and no impact on any results presented in ANL-EBS-MD-000037 REV 04 AD01.

Overall ERD Impact Evaluation:

Below is a list of AMR's that use ANL-EBS-MD-000037 REV 04 AD01 (DIRS# 180506) as a source: ANL-DS0-NU-000001 Rev. 00, ANL-EBS-GS-000001 Rev. 02, ANL-EBS-MD-000033 Rev. 06, ANL-NBS-HS-000057 Rev. 00, ANL-WIS-MD-000010 Rev. 06, ANL-WIS-MD-000024 Rev. 01, ANL-WIS-MD-000027 Rev. 00, ANL-WIS-PA-000001 Rev. 03, MDL-EBS-PA-000004 Rev. 03, MDL-WIS-PA-000005 Rev. 00, TDR-PCS-SE-000001 Rev. 05, Addendum 01, TDR-TDIP-NF-000007 Rev. 00, TDR-WIS-PA-000014 Rev. 00, DOE/EIS-0250-S1D, LASAR-2.03.07 and MDL-WIS-PA-000005 Rev. 00, Addendum 01. **There is no impact to any of these documents because there are no substantial text changes other than changes related to the DIRS numbers.**