Model
Error Resolution Document

Complete only applicable items.

QA:QA 11-20-08

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1. Document Number:	ANL-EBS-MD-000037	2. Revision/Addendum:	04/01	3. ERD:	02
4. Title:	In-Package Chemistry Abstraction				
5. No. of Pages Attached:	Attachment A: 3 pages; Attachment B: 3 pages				

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

This Error Resolution Document (ERD) addresses issues identified in condition report (CR) 12448 associated with model report *In-Package Chemistry Abstraction*, ANL-EBS-MD-000037 REV 04 AD 01.

CR 12448 identifies errors in two figures and a statement in the model report: (1) Figure 6-1[a] (p. 6-13[a]) contains data errors; (2) Figure 6-18[a] (p. 6-37[a]) contains a typographical error; and (3) a statement on p. 6-11[a] is erroneous due to the errors in Figure 6-1[a]. The data errors in Figure 6-1[a] prompted a minor revision of DTN: SN0702PAIPC1CA.001 (REV 003). Changes to the model report are made in this ERD to correct the figures and text, as described in Attachment A. No software controlled under IM-PRO-003, *Software Management*, was used for this ERD, and no changes were made to inputs.

The changes in this ERD do not impact the model abstractions or the overall model conclusion. Furthermore, they do not impact downstream controlled documents. A summary of the impact analysis is provided in Attachment B. The summary considers all controlled documents that cite the model report or its output DTN.

7. CONCURRENCE			
	Printed Name	Signature	Date
Checker	Susan Boggs		11/14/08
QCS/QA Reviewer	Peter Persoff		11/14/2008
8. APPROVAL			
Originator	Paul Mariner		11/19/2008
Responsible Manager	Robert MacKinnon		11/19/08

ATTACHMENT A

ANL-EBS-MD-000037 ERD 02 Corrections

A.1 Corrections in Response to CR 12448

CR 12448 identifies errors in two figures (Figures 6-1[a] and 6-18[a]) of *In-Package Chemistry Abstraction*, ANL-EBS-MD-000037 REV 04 AD 01 (SNL 2007 [DIRS 180506]). The error in Figure 6-1[a] is caused by an error in worksheet in revision 002 of Output DTN: SN0702PAIPC1CA.001. The error in Figure 6-18[a] is a typographical error in the report.

A.1.1 Figure 6-1[a]

The errors identified in Figure 6-1[a] are due to an error in the equilibrium constant used in column R of worksheet "CSNF Rate" of spreadsheet "Rates CSNF Cell 1.xls" in revision 002 of Output DTN: SN0702PAIPC1CA.001. According to the data0.ymp.R5 database (DTN: SN0612T0502404.014 [DIRS 178850]), the log of the equilibrium constant should be 7.81, not 6.34, for the reaction HCO_3^- + H^+ = $CO_2(g)$ + H_2O at 25°C. Output DTN: SN0702PAIPC1CA.001 was revised to correct this error. In addition, the 90°C calculations were improved in the worksheet in the DTN revision. Instead of using the 25°C equilibrium constants as approximations for the 90°C constants in columns R and S, more accurate constants for the reactions at 90°C, estimated by linear interpolation of the 60°C and 100°C data in the data0.ymp.R5 database, were incorporated, as documented in revision 003 of Output DTN: SN0702PAIPC1CA.001.

To correct the errors in the report associated with the worksheet errors described above and to synchronize the model report with the revised DTN, the following changes are made:

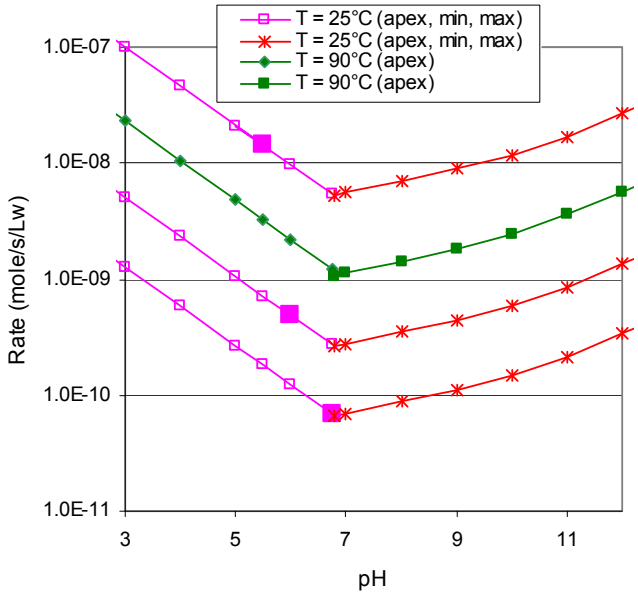
1. In Section 6.3.1.3.4[a] on p. 6-13[a], replace Figure 6-1[a] with Figure 6-1[a] of this ERD.
2. In Section 6.3.1.3.4[a] on p. 6-11[a] in the second full paragraph, remove the statement: "The discontinuities at pH 6.8 are due to the fitting functions used in the source."
3. In Section 6.3.1.3[a], in the notes of Tables 6-2[a], 6-3[a], and 6-7[a], and Figure 6-1[a], "Rates CSNF Cell 1.xls" is cited. Replace each citation with "Rates CSNF Cell 1 r003.xls".
4. In Sections 6.3.1[a], 6.5[a], and 6.6[a] there are seven locations (pages 6-7[a], 6-14[a], 6-22[a], 6-30[a], 6-34[a], 6-41[a], and 6-45[a]) where "IPC file key revision 2.xls" is cited. Replace each citation with "IPC file key revision 3.xls".

The impact of these changes is addressed in Attachment B.

A.1.2 Figure 6-18[a]

In Section 6.6.3[a] on p. 6-37[a], the lower left corner of Figure 6-18[a] contains text that indicates it represents results for the CSNF 2MCO Cell. This is a typographical error. The

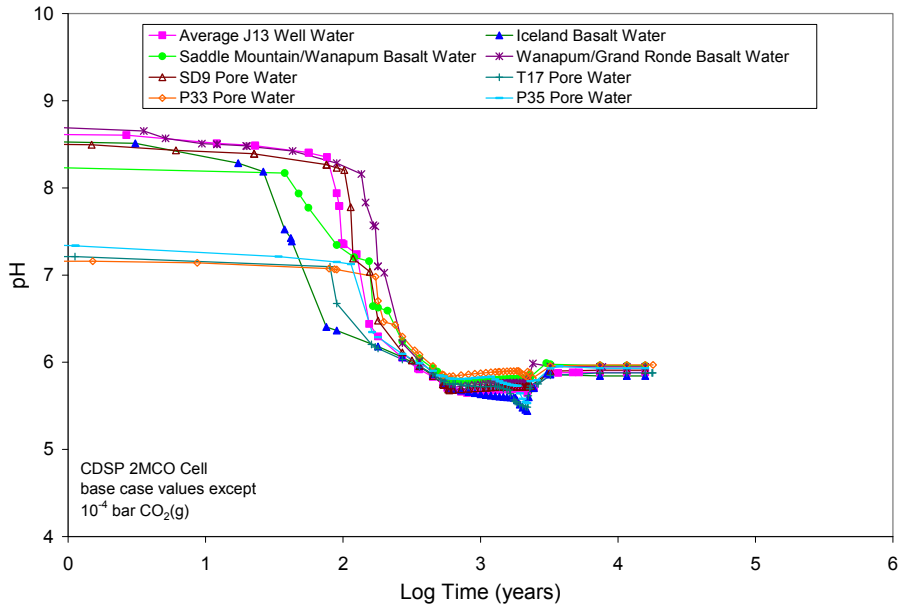
correct CDSP designation is documented in the source file. Replace “CSNF" with “CDSP” as shown in Figure 6-18[a] of this ERD. This change has no impact, as indicated in Attachment B.



Source: Output DTN: SN0702PAIPC1CA.001, file: *Rates CSNF Cell 1 r003.xls*.

NOTE: The minimum, maximum, and base case rates used in this addendum are marked by the large solid squares on the 25°C lines. Apex indicates most probable.

Figure 6-1[a]. CSNF Degradation Rate per Liter of Water (Lw) in the Liquid Influx Model



Source: Output DTN: SN0702PAIPC1CA.001, file: *2MCO low co2.xls*.

Figure 6-18[a]. 2MCO Liquid-Influx pH over Time for Various Seepage Compositions at 10^{-4} bar CO2(g)

ATTACHMENT B

ANL-EBS-MD-000037 ERD 02 Impact Analysis

B.1 Impact on Source Document

Changes to *In-Package Chemistry Abstraction*, ANL-EBS-MD-000037 REV 04 AD 01 (SNL 2007 [DIRS 180506]) resulting from CR 12448 are documented in Attachment A of this ERD. These changes affect two figures (Figures 6-1[a] and 6-18[a]), a statement related to Figure 6-1[a], and several cross references in the report. These changes do not affect the overall conclusion of the report and do not affect the associated DIRS report.

The change to Figure 6-18[a] is a minor editorial change. The change to Figure 6-1[a] is more substantive, but also minor because the erroneous values in the original figure are not used in any simulations of the report. The CSNF rates used in the report's simulations and abstractions are the three rates identified by the large solid squares in Figure 6-1[a], which are unaffected. These three values represent the minimum, maximum, and base case rates defined for the in-package chemistry simulations.

B.2 Impact on Downstream Documents

The changes listed in Attachment A of this ERD have no impact on downstream documents for the following reasons:

1. There is no impact to the overall model conclusion of *In-Package Chemistry Abstraction*, ANL-EBS-MD-000037 REV 04 AD 01.

2. Changes to the Output DTN of the report are minor and do not affect calculations that are used by downstream models and documents.

3. The changed figures are not cited or reproduced in downstream documents.

The changes made in this ERD are relevant only to the addendum, not the parent document. Therefore, the DIRS database was used to query all controlled downstream documents that cite REV 04 AD 01. This query resulted in the documents listed in Table B-1. As indicated in the table, the changes specified in Attachment A of this ERD have no impact on these downstream documents.

The controlled documents citing previous revisions (000, 001, and 002) of Output DTN: SN0702PAIPC1CA.001 were also determined from the DIRS database. These documents are listed in Table B-2. As indicated in the table, the changes have no impact on the controlled documents citing this DTN.

The License Application (LA) was also inspected for citations to the changed figures and calculations. No such citations were found; therefore, it is concluded that the changes in this ERD do not impact the LA.

The Yucca Mountain Repository Safety Analysis Report (SAR) was also inspected for impacts due to the changes implemented in this ERD. A scan of Section 2.3.7, titled *Waste Form Degradation and Mobilization and Engineered Barrier System Flow and Transport*, revealed no references to the text and figures changed in this ERD.

Table B-1. Controlled Documents That Cite REV 04 AD 01 and Relevance of Changes

DIRS	Document	Relevance of Changes
173869	SNL (Sandia National Laboratories) 2008. *Screening Analysis of Criticality Features, Events, and Processes for License Application.* ANL-DS0-NU-000001 REV 00.	Direct Input: none Indirect Input: not applicable
181165	SNL 2007. *Geochemistry Model Validation Report: Material Degradation and Release Model.* ANL-EBS-GS-000001 REV 02.	Direct Input: none Indirect Input: not applicable
177412	SNL 2007. *Engineered Barrier System: Physical and Chemical Environment.* ANL-EBS-MD-000033 REV 06.	Direct Input: none Indirect Input: not applicable
179962	SNL 2008. *Postclosure Analysis of the Range of Design Thermal Loadings.* ANL-NBS-HS-000057 REV 00.	Direct Input: none Indirect Input: not applicable
177418	SNL 2007. *Dissolved Concentration Limits of Elements with Radioactive Isotopes.* ANL-WIS-MD-000010 REV 06.	Direct Input: none Indirect Input: not applicable
177464	SNL 2008. *Postclosure Nuclear Safety Design Bases.* ANL-WIS-MD-000024 REV 01.	Direct Input: not applicable Indirect Input: not applicable
183041	SNL 2008. *Features, Events, and Processes for the Total System Performance Assessment: Analyses.* ANL-WIS-MD-000027 REV 00.	Direct Input: not applicable Indirect Input: not applicable
177407	SNL 2007. *EBS Radionuclide Transport Abstraction.* ANL-WIS-PA-000001 REV 03.	Direct Input: none Indirect Input: not applicable
177423	SNL 2007. *Waste Form and In-Drift Colloids-Associated Radionuclide Concentrations: Abstraction and Summary.* MDL-EBS-PA-000004 REV 03.	Direct Input: not applicable Indirect Input: not applicable
183478	SNL 2008. *Total System Performance Assessment Model /Analysis for the License Application.* MDL-WIS-PA-000005 REV 00 AD 01.	Direct Input: none Indirect Input: not applicable
	MDL-WIS-PA-000005 Rev. 00, MiscId 01 - Volume I	Direct Input: not applicable Indirect Input: not applicable
	MDL-WIS-PA-000005 Rev. 00, MiscId 02 - Volume II	Direct Input: none Indirect Input: not applicable
	MDL-WIS-PA-000005 Rev. 00, MiscId 03 - Volume III	Direct Input: none Indirect Input: not applicable
	MDL-WIS-PA-000005 Rev. 00, MiscId 08 - Volume III - 5	Direct Input: not applicable Indirect Input: not applicable
184797	SNL 2008. *Performance Confirmation Plan.* TDR-PCS-SE-000001 REV 05 AD 01.	Direct Input: none Indirect Input: not applicable
182846	SNL 2007. *TSPA Information Package for the Draft Supplemental Environmental Impact Statement.* TDR-WIS-PA-000014 REV 00.	Direct Input: none Indirect Input: not applicable

Table B-2. Controlled Documents That Cite Previous Revisions of Output DTN: SN0702PAIPC1CA.001 and Relevance of Changes

DIRS	Document	Relevance of Changes
177412	SNL 2007. *Engineered Barrier System: Physical and Chemical Environment.* ANL-EBS-MD-000033 REV 06.	Direct Input: none Indirect Input: not applicable
177418	SNL 2007. *Dissolved Concentration Limits of Elements with Radioactive Isotopes.* ANL-WIS-MD-000010 REV 06.	Direct Input: not applicable Indirect Input: not applicable
183041	SNL 2008. *Features, Events, and Processes for the Total System Performance Assessment: Analyses.* ANL-WIS-MD-000027 REV 00.	Direct Input: not applicable Indirect Input: none
183478	SNL 2008. *Total System Performance Assessment Model /Analysis for the License Application.* MDL-WIS-PA-000005 REV 00 AD 01.	Direct Input: none Indirect Input: not applicable
	MDL-WIS-PA-000005 Rev. 00, MiscId 01 - Volume I	Direct Input: not applicable Indirect Input: none
	MDL-WIS-PA-000005 Rev. 00, MiscId 02 - Volume II	Direct Input: none Indirect Input: not applicable
	MDL-WIS-PA-000005 Rev. 00, MiscId 03 - Volume III	Direct Input: not applicable Indirect Input: not applicable
	MDL-WIS-PA-000005 Rev. 00, MiscId 07 - Volume III - 4	Direct Input: not applicable Indirect Input: none
	MDL-WIS-PA-000005 Rev. 00, MiscId 08 - Volume III - 5	Direct Input: not applicable Indirect Input: none
182846	SNL 2007. *TSPA Information Package for the Draft Supplemental Environmental Impact Statement.* TDR-WIS-PA-000014 REV 00.	Direct Input: not applicable Indirect Input: none