



Model Error Resolution Document

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Complete only applicable items.

INITIATION

1. Originator: Ernest Hardin	2. Date: 03/18/2008	3. ERD No. ANL-EBS-MD-000033 ERD 01
4. Document Identifier: ANL-EBS-MD-000033 REV 06	5. Document Title: Engineered Barrier System: Physical and Chemical Environment	
6. Description of and Justification for Change (Identify applicable CRs and TBVs):		
<p>Introduction</p> <p>This document was created for the resolution of 3 TBV's (8783, 8784, and 8786) and 2 CR's (11849 and 11044). 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.</p> <p>1.) TBV-8784:</p> <p>Background Information Summary: Citation to [DIRS 179476] is incorrectly cited as SNL 2007 [DIRS 179476] instead of SNL 2008. Also, the wrong DIRS number was cited as [DIRS 179476] for DTN: MO0706SPAFAEPLA.001 should be [DIRS 181613].</p> <p>AMR changes:</p> <p>1.) Section 6.4 p. 6-74: revise the citation from DTN: MO0706SPAFAEPLA.001 [DIRS 179476] to MO0706SPAFAEPLA.001 [DIRS 181613].</p> <p>2.) Section 6.14, p. 6-245: revise the citation from SNL 2007 [DIRS 179476] to SNL 2008 [DIRS 179476] and add SNL 2008 [DIRS 183041] to the last sentence.</p> <p>3.) Section 9.1 p. 9-13: change reference as follows:</p> <p>179476 SNL 2008. <i>Features, Events, and Processes for the Total System Performance Assessment: Methods.</i> ANL-WIS-MD-000026 REV 00. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20080211.0010.</p> <p>Add reference as follows:</p> <p>183041 SNL 2008. <i>Features, Events, and Processes for the Total System Performance Assessment: Analyses.</i> ANL-WIS-MD-000027 REV 00. Las Vegas, Nevada: Sandia National Laboratories. DOC.20080307.0003.</p>		

CONCURRENCE

	Printed Name	Signature	Date
7. Checker	William Downs		3/27/08
8. QCS/QA Reviewer	Robert E. Spencer		3/27/08
APPROVAL			
9. Originator	Ernest Hardin		3/27/08
10. Responsible Manager	Paul Dixon		3-27-08



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

Impact Evaluation: The change to the year and the addition of [DIRS 183041] is reflected on a corrected final DIRS report for ANL-EBS-MD-000033 REV 06. There is no impact on the conclusions of the AMR from this minor editorial change.

2.) TBV-8786:

Background Information Summary: SNL 2007 [DIRS 179354] was incorrectly cited for the Repository design information, waste package end-point coordinates, the citation should be to SNL 2007 [DIRS 179466]. The information is correctly cited, only the DIRS number was incorrect.

AMR changes:

1.) Table 4.1-1, p. 4-3 (first row, last entry for parameter 02-01): The citation for "Repository design information, waste package end-point coordinates"; should be changed from (SNL 2007 [DIRS 179354], Parameter Number 02-01) to (SNL 2007 [DIRS 179466], Table 4-1, Parameter Number 01-01).

2.) Section 4.1.10, p. 4-14: Changed as follows:

Waste package end-point locations are taken from *Total System Performance Assessment Data Input Package for Requirements Analysis for Subsurface Facilities* (SNL 2007 [DIRS 179466], Table 4-1, Parameter Number 01-01).

3.) Section 9.1: Add SNL 2007 [DIRS 179466] as follows:

179466 SNL 2007. *Total System Performance Assessment Data Input Package for Requirements Analysis for Subsurface Facilities*. TDR-TDIP-PA-000001 REV 00.
Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070921.0007.

4.) Figure 6.3-5: Changed as follows (Note that it was noticed that the figure was an old figure and is being corrected here as well):



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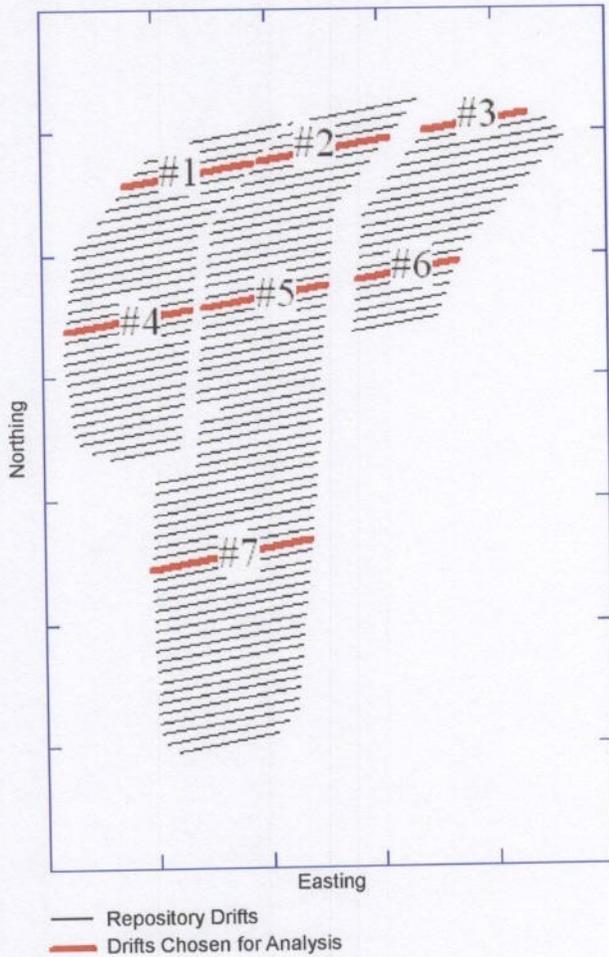
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NOTE: Drifts defined on the basis of waste package end-point coordinates in SNL 2007 [DIRS 179466], Table 4-1, Parameter Number 01-01.

Figure 6.3-5. Representative Repository Drift Locations Selected for the NFC Model



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6. Description of and Justification for Change (Identify applicable CRs and TBVs) Continued:
Inputs and/or Software: Change to DIRS numbers as stated above, but no changes to any information used.

Impact Evaluation/Results: The changes are reflected on a corrected final DIRS report for ANL-EBS-MD-000033 REV06. There is no impact on the conclusions of the AMR, the information is correctly cited, only the DIRS number was incorrect.

3.) TBV- 8783:

Background Information Summary: There were several instances where the information that directs the user to SNL 2007 [DIRS 177407], was not traceable as cited in the AMR. The changes are being made to make the citation more transparent and traceable.

AMR changes:

1.) Table 4.1-1, p. 4-4 (12th row): Changed row as follows:

SNL 2007 [DIRS 177407]	Corrosion product porosity	Section 6.3.4.3.4.2
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2.) Table 4.1-17 p. 4-28 (3rd to last row and last row): Changed rows as follows:

Corrosion product porosity	0.4	th7_81_GasCalc_Invert June2007.xls, th7_162_GasCalc_Invert June2007.xls	SNL 2007 [DIRS 177407], Section 6.3.4.3.4.2
Chosen specific surface areas of steel corrosion products	1 m ² /g and 22 m ² /g	Deff (RTA based) May2007.xls	SNL 2007 [DIRS 177407], Table 6.3-7 (range in Fe ₂ O ₃)

3.) Section 6.7.1.5, p. 6-126: Changed as follows:

ϕ_{CP} = Corrosion product porosity (40%; see SNL 2007 [DIRS 177407], Section 6.3.4.3.4.2).

4.) Section 6.7.1.5, p. 6-126: The following statement was cited from DIRS 177407 :

For in-package transport of radionuclides by diffusion through corrosion products, a set of moisture characteristic curves (liquid saturation vs. RH) and effective liquid-phase diffusion coefficients (*Deff* vs. liquid saturation) was developed (SNL 2007 [DIRS 177407], Table 6.3-10).

Background

This statement above could not be verified as written: The following analysis should be added to Section 6.7.1.5, p. 6-126 as an explanation of the use of the set of moisture characteristic curves (liquid saturation vs. RH) and effective liquid-phase diffusion coefficients (*Deff* vs. liquid saturation):



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

The oxygen consumption analysis relies on moisture characteristic curves for corrosion products, from a previous revision of *EBS Radionuclide Transport Abstraction* (BSC 2005 [DIRS 173433], Table 6.3-10, herein called the previous revision). These curves do not appear in the current revision (SNL 2007 [DIRS 177407]; Section 6.3.4.2.3.1) which is expanded to include additional data from the technical literature, and to represent an assemblage of products that is likely to result from degradation of stainless steel.

This is an evaluation of whether information from the previous revision still leads to appropriate conclusions from the oxygen consumption analysis, in light of the updated information from the current revision.

Analysis (also to be added to Section 6.7.1.5):

The oxygen consumption analysis uses the specific surface area and effective aqueous diffusion coefficient information from (BSC 2005 [DIRS 173433]), in the second part, which evaluates the effect from diffusive mass transfer of molecular O₂ through a layer of corrosion products. The changes in source information have no impact on the first part, which analyzes the effects from oxygen consumption based only on intrinsic kinetic limitations, without mass transfer limitations. The mass transfer analysis (second part) supports the conclusions based on the first part (Section 6.7.1.7).

The discussion below shows that use of larger values of specific surface area in the analysis tends to further moderate the intensity of oxygen depletion, fully consistent with the conclusion of the analysis that chemically oxidizing conditions will be maintained in the EBS environment (Section 6.7.1.7). The current information with greater specific surface area for corrosion products leads to greater liquid saturation, which impedes gas-phase O₂ transport, moderating the corrosion rate, and supporting the conclusion of the oxygen consumption analysis.

Two types of information were obtained from the previous revision (BSC 2005 [DIRS 173433], Table 6.3-10): 1) a moisture characteristic curve (also called water retention curve, expressed as liquid saturation vs. relative humidity), and 2) effective liquid-phase diffusion coefficient for dissolved species (versus relative humidity). The characteristic curve was generated using a water sorption isotherm for hematite (expressed as layers of water molecules vs. relative humidity) multiplied by the ratio of surface area to pore volume, to determine the fraction of pore volume filled with liquid (SNL 2007 [DIRS 177407], Section 6.3.4.3.5). Available isotherms for water sorption on hematite, goethite, HFO, and other phases likely to form tend to lie within a relatively narrow range (SNL 2007 [DIRS 177407], Figure 6.3-34) over which the effect on the characteristic curve is small compared to the uncertainty in specific surface area of steel corrosion products (represented by the range of data reported in SNL 2007 [DIRS 177407], Tables 4.1-12 and 4.1-14). Note that porosity of corrosion products (representing pore volume) is taken in both the previous and current revisions to be 40% (SNL 2007 [DIRS 177407], p. 6-93).

The impact of the current revision on the moisture characteristic curve from the previous revision is thus mainly due to the extended range of specific surface area reported for corrosion products. Greater specific surface area means more water is sorbed at a given humidity, increasing the liquid saturation, and decreasing the gas saturation. Diffusive transport of O₂ in partially saturated granular materials is dominated by the gas phase,



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

because the diffusion coefficient is several orders of magnitude greater than in liquid water. Diffusion of O₂ in liquid water is bounded by the self-diffusion coefficient of water (nominally 2.299×10^{-9} m²/sec; SNL 2007 [DIRS 177407], p. 6-40) compared to the binary diffusion coefficient for O₂ in air (nominally 2.10×10^{-4} m²/sec; SNL 2007 [DIRS 177412], Table 4.1-17).

The effective diffusion coefficient through liquid water-filled porosity in granular media is represented by Archie's law (SNL 2007 [DIRS 177407], Section 6.3.4.3.5), and is directly related to porosity and liquid saturation. Effective coefficients for aqueous diffusion obtained from the previous revision (BSC 2005 [DIRS 173433], Table 6.3-10) were calculated from liquid saturation (and are not independently developed). Increased saturation produces increased aqueous diffusion, but greatly decreased gas-phase diffusion, and thus overall greatly decreased diffusion of O₂ in corrosion products at partial saturation. In summary, the impact of the current revision, on both types of information obtained from the previous revision, is dominated by the wider range of specific surface area and the resulting decrease in the overall effective diffusion of O₂ in corrosion products.

The impact of decreased overall effective diffusion on the oxygen consumption analysis is negligible. This can be verified using the Excel spreadsheet that implements the analysis, specifically the second part of the analysis that implements mass transfer in addition to intrinsic kinetics (output DTN: MO0705OXYBALAN.000, File: *th7_81_GasCalc_Invert_June 2007.xls*, Worksheet: *O2 Calc. with Mass Transfer*). Cell A27 of this worksheet is a multiplier supplied for use in sensitivity testing, and applied to both the aqueous and gas-phase effective diffusion coefficients. The analysis is performed using a value of one in this cell. However, large changes in this multiplier do not significantly change the range of results shown in the plotted histories of O₂ pressure, although some of the uncertainty cases can shift. This insensitivity is due partly to the greater importance of intrinsic kinetics.

Impact Summary

The information obtained from the previous revision is valid and not associated with any known errors. It has been replaced with a wider range of data, particularly greater values for specific surface area of Fe-bearing steel corrosion products (SNL 2007 [DIRS 177407], Tables 4.1-12 and 4.1-14). Greater specific surface area produces greater liquid saturation, which decreases the overall diffusive transport of O₂ in corrosion products at partial saturation. This tends to moderate the rate of consumption of O₂ in the analysis that includes both mass transfer and intrinsic kinetics (SNL 2007 [DIRS 177412], Section 6.7.1.5). The effect on the postclosure range of variation for O₂ partial pressure calculated for the emplacement drifts is negligible, and the conclusion of the analysis is unaffected.

5.) Section 6.7.1.5, p. 6-126: The two values of specific surface area (1 m²/g and 22 m²/g) from *EBS Radionuclide Transport Abstraction* (SNL 2007 [DIRS 177407], Table 6.3-7 (range in Fe₂O₃)) are used in this analysis.



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

6.) **Section 6.7.1.5, p. 6-126, 3rd paragraph 3rd sentence** changed as follows: Considerably larger values of specific surface area are possible, as indicated in *EBS Radionuclide Transport Abstraction* (SNL 2007 [DIRS 177407], Section 6.3.4.3.3).

7.) **Section 6.15.2: p. 6-258** changed as follows: (1) condensate is benign to waste package localized corrosion (see SNL 2007 [DIRS 177407], Section 6.3.3.2.5);

Inputs and/or Software: No changes.

Impact Evaluation/Results: The changes are reflected on a corrected final DIRS report for ANL-EBS-MD-000033 REV06. There is no impact on the conclusions of the AMR, the information is correctly cited but needed additional information to be more transparent and traceable.

4.) **CR-11849:** Editorial Changes to ANL-EBS-MD-000033 REV06.

Background Information Summary: After the P&CE report (SNL 2007 [DIRS 177412]) was submitted to and accepted by DOE, several editorial errors were discovered. The purpose of CR-11849 is to capture all of the known errors such that they may be resolved to improve quality and traceability of the report.

AMR changes:

1.) **Table 4.1-17:** The units are missing from the binary diffusion coefficient of O₂ in air at 25C. The second column should read 2.10x10⁻⁴ m²/s.

2.) **Figure 6.6-18:** The Figure caption should be changed to read: Change in Chloride: Nitrate Molal Ratio with Evaporation.

3.) **Section 6.8.3, 6-147:** In the paragraph right before Section 6.8.4; the paragraph begins: A parametric sensitivity to this corrosion rate.....the last sentence contains an incorrect call-out. Change "Section 6.8.4.3" to "Section 6.8.4.2".

4.) **Section 7.1.1.4, p. 7-14:** In the first two paragraphs all units should be mol sec⁻¹ kg tuff¹ (moles per second per kg tuff) in some instances the units are incorrectly reported as mol yr⁻¹ kg tuff¹.

5.) **Section 7.1.4, p. 7-38:** The first paragraph on the page, third sentence change "water packages" to "waste packages".



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6) **Section 6.15.1, p. 6-251:** Add a clarifying sentence at the end of the paragraph right before Fig. 6.15-2: "This is accomplished by linearly scaling between ambient and the minimum or maximum using the absolute value of $\Delta p\text{CO}_2$ as the scaling factor."

7) **Table 8.2-1:** One of the output DTNs that provides data to the TSPA is missing from the table. Added as follows:

SN0706PAEBSPCE.016	Sections 6.9.4 and 6.15.2.1	"This DTN contains EQ3/6 simulations of dilute water interactions with rock minerals. These simulations form the basis for the RH boundary limit on invert dilution."
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8) **Section 6.12, p. 6-189 through 6-191:** There are several sub-sections headings that are mis-numbered. On **page 6-189** change the sub-section number from 6.12.2.2 to 6.12.2.2.2; on **page 6-190** sub-section number 6.12.2.3 should be 6.12.2.2.3; on **page 191** sub-section number 6.12.2.4 should be 6.12.2.2.4; also on **page 6-191** sub-section number 6.12.2.5 should be 6.12.2.2.5.

9) **pp. 6-37, 6-39, 6-45, 6-106 and 6-252:** Related to number (8) above, several call-outs in the text must be corrected: on **page 6-37** at the bottom the call-out to Section 6.12.2.1 should be Section 6.12.2.2.1; on **page 6-39** in two locations Section 6.12.2.1 should be Section 6.12.2.2.1; on **page 6-45** the paragraph just after equation 6.3-18 the call-out to Section 6.12.2.1 should be Section 6.12.2.2.1; on **page 6-106** at the top right before Figure 6.6-13 the call-out to Section 6.12.2.1 should be Section 6.12.2.2.1; on **page 6-252** the call-out to Section 6.12.2.5 should be Section 6.12.2.2.5.

10) **Section 1:** In the first bulleted point on page 1-2: Change the paragraph so that the last sentence reads: "While DST data are evaluated in the NFC post-development model validation, the applicability of these data is limited because the relatively short time scale represented by the DST limited the degree of water-rock interaction."

11) **Section 6.12.4.2, p. 6-215:** There are errors in the formatting of " $p\text{CO}_2$ " (Should be $p\text{CO}_2$ not $p\text{CO}2$).

12) **Table 6.2-3, p. 6-23:** The kogarkoite formula is incorrect and should be $\text{Na}_3\text{SO}_4\text{F}$.

13) **Section 6.15.1 p 6-255:** Change the third sentence of the last paragraph to read: "When selecting chemical parameters that fall between lookup tables, the parameters should be estimated using linear interpolation on temperature and WRIP value, and log linear interpolation for $p\text{CO}_2$ parameters."



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Impact Evaluation/Results: There were no changes needed for the DIRS report for ANL-EBS-MD-000033 REV06. There is no impact on the conclusions of the AMR, the information is correctly cited but needed either an editorial change or additional information to be more transparent and traceable.

Inputs and/or Software: No changes.

Other minor editorial corrections (extent of the condition for CR 11849):

- 1.) Section 6.7.1.4, p. 6-122: There is an error for $R = \text{Gas constant}$ in the formatting of " $\text{Pa m}^3/\text{mol-K}$ ". (should be $\text{Pa m}^3/\text{mol-K}$ not $\text{Pa m}^3/\text{mol-K}$).
- 2.) Section 6.7.1.4 p. 6-123: replace "." with "," in the value for ρ_{steel} the density of steel (should be 7,850 not 7.850).

Impact Evaluation/Results: There were no changes needed for the DIRS report for ANL-EBS-MD-000033 REV06. There is no impact on the conclusions of the AMR, the information is correctly cited but needed either an editorial change or additional information to be more transparent and traceable.

5.) CR-11044: IDPS (ANL-EBS-MD-000045 REV 03) Pitzer Database (DTN SN0609T0502404.012) Area to Improve and Potential Limitation.

Background Information Summary: The DTN SN0609T0502404.012 [DIRS 179067] was used as an input into ANL-EBS-MD-000033 REV 06. To evaluate any impact of this issue within the ANL-EBS-MD-000033 REV 06, each spreadsheet lookup table was examined for a(w) reversals.

Inputs and/or Software: No changes.

AMR changes: No changes.

Impact Evaluation/Results: Reversals were found in six spreadsheets (20p2t1.xls, 20p3t30.xls, 20p4t1.xls, 20p4t30.xls, 2bp2t30.xls, and 2jp2t1.xls) from downstream source DTN: SN0609T0502404.012 [DIRS 179067]. In addition, a sharp uncharacteristic change was observed at the end of 2ip4t70.xls. The README file in output DTN: SN0701PAEBSPCE.001 has been updated noting that these a(w) reverses occur in spreadsheets 20p2t1.xls, 20p3t30.xls, 20p4t1.xls, 20p4t30.xls, 2bp2t30.xls, 2jp2t1.xls, and 2ip4t70.xls and that these simulations should be truncated where a(w) begins to increase. For these seven spreadsheets, none of these reversals/changes occurred at a(w) values greater than 0.66 (i.e. $\text{RH} > 66\%$). The seven lookup tables generated from these are used within TSPA to determine conditions for initiation of corrosion on the drip shield and waste



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package, and to determine the aqueous composition in the invert. Because the aqueous composition in the invert is only relevant at 95% RH or higher; these a(w) reversals have no effect on modeling in the invert. For use in corrosion evaluation, it is noted that none of the seven tables noted above were sampled in the RH range (<66%) of the condition except perhaps for a single time step that might have been used when the RH was right at 66% (See CR 11044 attached file "CR 11044 Zwahlen e-mail.pdf"). Therefore, this truncation does not affect results used by TSPA.

Overall ERD Impact Evaluation:

Below is a list of AMR's that use ANL-EBS-MD-000033 REV 06(DIRS 177412) as a source:

ANL-EBS-GS-000001 Rev. 02, ANL-EBS-MD-000003 Rev. 03, ANL-EBS-MD-000004 Rev. 02, Addendum 01, ANL-EBS-MD-000037 Rev. 04, Addendum 01, ANL-EBS-MD-000049 Rev. 03, Addendums 01 and 02, ANL-NBS-HS-000047 Rev. 01, 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-MD-000001 Rev. 00, Addendum 01, MDL-EBS-PA-000004 Rev. 03, MDL-NBS-HS-000001 Rev. 05, MDL-NBS-HS-000020 Rev. 02, Addendum 01, MDL-WIS-PA-000005 Rev. 00, TDR-PCS-SE-000001 Rev. 05, Addendum 01, TDR-TDIP-NF-000005 Rev. 00, TDR-TDIP-NF-000006 Rev. 00, TDR-TDIP-NF-000007 Rev. 00, TDR-TDIP-NS-000003 Rev. 00, TDR-WIS-PA-000014 Rev. 00, DOE/EIS-0250-S1D MiscId 17, LASAR-2.03.04, LASAR-2.03.05, and LASAR-2.03.06. **There is no impact to any of these documents because there are no substantial text changes other than changes related to the DIRS numbers.**