Model Error Resolution Document	
Complete only applicable items.	QA: QA Page 1 of 50

1. Document Number: ANL-WIS-PA-000001	**2. Revision/Addendum:** REV 03	**3. ERD:** 02
4. Title: EBS Radionuclide Transport Abstraction	**5. No. of Pages Attached:** 49	

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

This Error Resolution Document (ERD) addresses issues identified in eight condition reports (CRs) associated with analysis/model report *EBS Radionuclide Transport Abstraction*, ANL-WIS-PA-000001 REV 03 [DIRS 177407], None of the changes documented in this ERD has any impact upon the conclusions of ANL-WIS-PA-000001 REV 03, nor on any downstream citation of ANL-WIS-PA-000001 REV 03, including the License Application (LA), the Final Environmental Impact Statement (FEIS), or the Supplemental Environmental Impact Statement (SEIS).

1) CR 12867 identifies a number of typographical errors, omissions, and needed clarifications in ANL-WIS-PA-000001 REV 03. Resolution of CR 12867 is addressed in Section I.

2) CR 12998 concerns the model for radionuclide sorption onto corrosion products that is developed in ANL-WIS-PA-000001 REV 03. In certain cases, the model may overestimate sorption of radionuclides, thereby underestimating releases. Resolution of CR 12998 is addressed in Section II.

3) CR 13093 identifies repository design data in ANL-WIS-PA-000001 REV 03, Section 4 and Appendix I, that are incorrectly referenced to certain tables in the design TSPA Data Input Package (TDIP) documents. The data are not found in the cited tables, but rather in other tables and figures in the design TDIPs. Resolution of CR 13093 is addressed in Section III.

4) CR 10788 addresses a procedural non-compliance regarding qualification of external source data used as direct input. A review of ANL-WIS-PA-000001 REV 03 revealed that most of the information required for the qualification of external data was presented in the document, but some of the documentation requirements of SCI-PRO-001, *Qualification of Unqualified Data*, were omitted. Resolution of CR 10788 is addressed in Section IV.

5) CR 13657 identifies incorrect references in Figures 7.2-13 and 7.2-14. Resolution of CR 13657 is addressed in Section V.

6) CR 13740 identifies errors in describing the concentration of competing cations in the validation of the competitive surface complexation model in ANL-WIS-PA-000001 REV 03, Section 7.2.3. Concentrations characterized as "highest" should be "lowest." Resolution of CR 13740 is addressed in Section VI.

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7) CR 13678 identifies two figures, Figures 6.5-10 and 6.5-11, in ANL-WIS-PA-000001 REV 03, Section 6.5.2.4.6 that contain illegible figure and axis labels. These figures are a matrix of plots shown together, but are of a very poor resolution. Resolution of CR 13678 is addressed in Section VII.

8) CR 13643 indicates that Eq. 6.5.1.2-9, p. 6-149, which describes the rate of formation of "embedded" colloids, incorrectly uses the aqueous concentration and should instead use the total concentration that includes the mass in all phases, both aqueous and stationary. Resolution of CR 13643 is addressed in Section VIII.

I. CR 12867 Resolution

In CR 12867, file "EBS RTA REV03 Typos 2008[1].doc" identifies 39 typographical errors, omissions, or clarifications needed in ANL-WIS-PA-000001 REV 03. In this section, 33 of those issues are addressed. The remaining 6 issues have been addressed in response to other CRs. Specifically, Item 16 in the CR 12867 file mentions that addition of a description of how parameter Diff_Path_Length_Invert_Top_a is computed on p. 6-191, following Eq. 6.5.2.3-5, would improve transparency; this issue was resolved in ANL-WIS-PA-000001 REV 03 ERD 01, pp. 6 – 8, in response to CR 11816. Item 15 in the CR 12867 file concerns a typographical error in reporting the ranges of this parameter on p. 8-18, Table 8.2-4; this was also resolved in ANL-WIS-PA-000001 REV 03 ERD 01, pp. 6 – 8, in response to CR 11816. Four other typographical errors involving FHH parameters (Items 11 – 14 in the CR 12867 file) were corrected in ANL-WIS-PA-000001 REV 03 ERD 01, pp. 6 – 8, in response to CR 11755.

CR 12867 is resolved by the following 33 changes (in which underlining indicates the original text to be changed and the revised text) to ANL-WIS-PA-000001 REV 03. Seven additional changes (#34 – #40) clarify text or correct errors that were identified subsequent to CR 12867 being issued. None of these changes impacts the conclusions of the document, and no downstream usage—neither the LA nor other project documents—is impacted. Changes to the DIRS that are noted below are marked up on the point-in-time DIRS report, and the revised DIRS report is processed in accordance with SCI-PRO-004, *Managing Technical Product Inputs*; the marked-up pages from the DIRS report are appended to this ERD.

1. p. 4-47, Table 4.1-20: Add row under "TAD Canister and Waste Package Characteristics" for: "Inner vessel length, 216.50 in., SNL 2007 [DIRS 179394], Table 4-3." This parameter is used on p. 6-166, Section 6.5.2.1.1.2, to compute the diffusive area for the path excluding the outer barrier, parameter Diff_Area_CSNF_2, of 29.9 m^2. The DIRS entry for SNL 2007 [DIRS 179394] in the DIRS list for ANL-WIS-PA-000001 REV 03 is modified to include this particular direct input, as follows:

DIRS entry for SNL 2007 [DIRS 179394] for ANL-WIS-PA-000001 REV 03

Table 4-3	Section 6.3.3.2.3;Tables 4.1-20 and 6.5-5	Outer corrosion barrier outside diameter; inner vessel outside diameter; outer corrosion barrier length; outer barrier thickness; outer lid thickness; inner vessel thickness	Direct Input	N/A	N/A	TBV-8615 Resolved

Revised DIRS entry for SNL 2007 [DIRS 179394] for ANL-WIS-PA-000001 REV 03 ERD 02

Table 4-3	Section 6.3.3.2.3;Tables 4.1-20 and 6.5-5	Outer corrosion barrier outside diameter; inner vessel outside diameter; outer corrosion barrier length; outer barrier thickness; outer lid thickness; inner vessel thickness; inner vessel length	Direct Input	N/A	N/A	TBV-8615 Resolved

2. p. 4-47, Table 4.1-20, 4th row from bottom: For entry "TMI canister guide tube cross section width," change source "p. 25" to "p. 30." This parameter is used in the output DTN: SN0703PAEBSRTA.001, file *5-DHLW-SNF DOE Long + TMI SNF + 21-PWR TAD 9-19-2007 Final TDIP.xls*, worksheet "5-DHLW-DOE Long + TMI SNF" to estimate masses of steels and corrosion products reported in Table 6.3-9 on pp. 6-88 – 6-89, Section 6.3.4.3.4.1. The DIRS entry for DOE 2003 [DIRS 164970] in the DIRS list for ANL-WIS-PA-000001 REV 03 is modified to include this particular input, which had not been listed. In addition, the input usage is revised to be Direct Input, rather than Indirect Input, since the inputs in this DIRS entry are used to obtain parameter Mass_Steel_CDSP_1b used in the TSPA. The DIRS entry is revised as follows:

DIRS entry for DOE 2003 [DIRS 164970] for ANL-WIS-PA-000001 REV 03

p. 30	Table 4.1-20	DSNF Characteristics - TMI canister guide tube length	Indirect Input	N/A	N/A	N/A

Revised DIRS entry for DOE 2003 [DIRS 164970] for ANL-WIS-PA-000001 REV 03 ERD 02

p. 30	Table 4.1-20	DSNF Characteristics - TMI canister guide tube length; TMI canister guide tube cross section width	Direct Input	Data	Qualified	N/A

3. p. 4-49, Table 4.1-22: Clarify that there are two different spread rings in the waste package: Change (3rd row) "Spread Ring" to "TAD Canister Spread Ring" and change (12th row) "Spread Ring" to "Waste Package Spread Ring." (The DIRS entry for the cited reference is not impacted because it does not identify individual waste package components.)

4. p. 6-6, bullet number 4, last line: Change "6.3.3.3)." to "6.3.3.2.5)."

5. p.6-19, 1st paragraph, line 5: Delete "A model of advective flow of water through stress corrosion cracking (SCCs) is presented in Section 6.3.3.1." (A SCC advective flow model is presented in the cited FEP, but not in ANL-WIS-PA-000001 REV 03.)

6. p.6-19, 1st paragraph, line 5: Change "6.3.3.3" to "6.3.3.2.5."

7. p.6-19, 1st paragraph, line 6: Change "6.3.3.4" to "6.3.3.3."

8. p.6-19, 1st paragraph, last line: Change "6.3.3.5" to "6.3.3.4." (Note: there is no section 6.3.3.5.)

9. p. 6-19, last line; p. 6-20, 1st 2 lines: Change "The TAD canister design has not been finalized; for purposes of estimating the masses of internal components, the Site-Specific Canister design is used for the TAD canister design (see Table 4.1-21 for a complete list of drawings used in this report)." to "The TAD canister design was not finalized until after analyses discussed in this report were completed; for purposes of estimating the masses of internal components, the Site-Specific Canister design was used for the TAD canister design (see Tables 4.1-20, 4.1-21, and 4.1-22 for a complete list of EBS component design information, component dimensions, and component masses and numbers, respectively, that are used in this report; see Table 4.1-23 for comparisons of component masses used in this report with final design values)."

10. p.6-20, Section 6.3.3.2, 1st paragraph, line 4: Change "Sections" to "Section."

11. p.6-27, Section 6.3.3.2.5, 1st paragraph, line 2: Change "thorough" to "through."

12. p.6-28, 1st paragraph after Equation 6.3.3.2.5-1, last line: Change "6.3.3.2.4" to "6.3.3.2.5." (Note: flow through stress corrosion cracks is not discussed until 6.3.3.2.5.)

13. p. 6-87, line 1: Change "6.3.3.1.1" to "6.3.3.1." (Note: there is no section 6.3.3.1.1.)

14. p. 6-88, Table 6.3-8: Clarify that there are 2 different spread rings in the waste package—one between the TAD shield plug and outer seal plate, the other between the inner top lid and outer (Alloy 22) lid. Change footnote b from "…Inner Seal Plug, Spread Ring, Spread Ring Filler Segment, …, Inner Top Lid, Inner Bottom Lid" to "…Inner Seal Plug, TAD Spread Ring, Spread Ring Filler Segment, …, Inner Top Lid, Overpack Spread Ring, Inner Bottom Lid."

15. p. 6-90, end of 1st paragraph: Change "approximately 1196 m^2" to "approximately 1195 m^2" (to be consistent with value reported in Table 6.3-10).

16. p. 6-90, 2nd paragraph, lines 2-7: Change "The volume inside the 21-PWR TAD waste package overpack outer corrosion barrier is calculated from dimensional data given in SNL 2007 [DIRS 179394], Table 4-3: The outer corrosion barrier outside diameter is 1.8816 m and thickness is 0.0254 m. The inside length is estimated from the inner vessel length of 5.4991 m and total outer corrosion barrier-inner vessel end-to-end gaps of 0.1128 m, which give an inside volume of 14.77 m^3 for the overpack. Then the initial void volume is 7.99 m^3" to "The volume inside the 21-PWR TAD waste package overpack outer corrosion barrier is

calculated from the following dimensional data given in SNL 2007 [DIRS 179394], Table 4-3: The outer corrosion barrier outside diameter is 1.8816 m and the wall thickness is 0.0254 m, so the outer corrosion barrier inside diameter is 1.8308 m. The outer corrosion barrier inside length is estimated by summing the enclosed inner vessel length of 5.4991 m, the outer corrosion barrier-inner vessel end-to-end top gap of 0.0445 m, and the outer corrosion barrier-inner vessel end-to-end bottom gap of 0.0683 m, for a total inside length of 5.6119 m. With these dimensions, the cylindrical overpack outer corrosion barrier has an inside volume of 14.77 m^3. Then, subtracting the volume of solid components contained within the overpack (6.82 m^3, from Table 6.3-10), the initial void volume is 7.95 m^3." (Note that the initial average porosity of 0.54 reported at the end of this sentence is unchanged by this correction.)

17. p. 6-91, Table 6.3-10: Change fuel rod total surface area "636.93" to "636.94." (Note: the calculation following Table 6.3-10, footnote d, gives 636.9367, correctly rounded to 636.94.)

18. p. 6-91, Table 6.3-10: Entry for Total Volume of Fuel Basket C-Plate needs to be aligned with rest of column; entries in Total Mass column for Spread Ring, Outer Seal Plate, and Total need to be aligned with rest of column. (Total value is misaligned due to footnote superscript; the number should be right-aligned, with footnote superscript extending beyond alignment to the right.)

19. p. 6-91, Table 6.3-10: Since *all* of the Total Mass values are the preliminary values listed in Table 4.1-23, delete the footnote f on Component names in the Component column as well as footnote f itself. In footnote a referring to Total Mass values, change "SNL 2007 [DIRS 179394], Tables 4-3 and A-1, except for preliminary values listed in Table 4.1-23." to "Preliminary values listed in Table 4.1-23." The DIRS entries are revised as follows (new DIRS entries are not shown in the appended DIRS mark-up but are listed in Attachment I):

DIRS entries for SNL 2007 [DIRS 179394] for ANL-WIS-PA-000001 REV 03

Table 4-3	Section 6.3.4.3.4.2	The volume inside the 21 PWR TAD waste package overpack outer corrosion barrier	Indirect Input	N/A	N/A	TBV-8615 Resolved
Table 4-2	Tables 4.1-21 and 6.5-5; Section 6.3.4.3.4.2	Component Dimensions in a 21-PWR Site-Specific Canister	Direct Input	N/A	N/A	TBV-8615 Resolved

Revised/new DIRS entries for SNL 2007 [DIRS 179394] for ANL-WIS-PA-000001 REV 03 ERD 02

Table 4-3	Section 6.3.4.3.4.2	Dimensional data for a 21 PWR TAD waste package overpack outer corrosion barrier	Indirect Input	N/A	N/A	TBV-8615 Resolved

Table 4-2	Tables 4.1-21 and 6.5-5	Component Dimensions in a 21-PWR Site-Specific Canister	Direct Input	N/A	N/A	TBV-8615 Resolved
Tables A-1 and A-3	Section 6.3.4.3.4.2; Table 6.3-10	Typical measurements and surface areas for 21-PWR TAD waste package components	Indirect Input	N/A	N/A	N/A

20. p. 6-143, full line before Equation 6.5.1.1.3-1: Change "6.3.3.3" to "6.3.3.2.5."

21. p. 6-143, last full paragraph (starting with "As with the drip"), last sentence: Change "to 1.022 m –or a 5- DHLW" to "to 1.022 m for a 5-DHLW." (Note: no space after "5-.")

22. p. 6-163: Change bold heading "**CSNF Waste Packages Properties**" to section heading "**6.5.2.1.1 CSNF Waste Packages Properties**." (Since the Table of Contents lists sections only to three levels, e.g., 6.5.2, this change does not impact the Table of Contents.)

23. p. 6-166, 2nd full paragraph (starting with "The diffusive areas"), 3rd line: Change "(radius of 0.819 m, from Section 2.4.2.1)" to "(radius of 0.819 m, from outside diameter of 66.5 in. (SNL 2007 [DIRS 179394], Section 4.1.1.1); and 1.00 in. thickness, (SNL 2007 [DIRS 179394], Table 4-2))." (The DIRS entries for this reference in the DIRS list for ANL-WIS-PA-000001 REV 03 are not impacted because these same data are cited and used in the same way in the preceding paragraph in this section.)

24. p. 6-174, Table 6.5-5, 6th row from bottom: Change heading "Component and Source" to be centered instead of left-justified.

25. p. 6-176, Table 6.5-7, Comments for Specific surface area of NiO and Cr_2O_3: Change "Based on data in Table 6.3-10" to "Based on data in Table 6.3-7" (changes in 2 rows).

26. p. 6-180, Figure 6.5-4 caption: Delete "Constant RH." (Plot is water saturation as a function of RH.)

27. p. 6-181, Figure 6.5-5 caption: Delete "Constant RH." (Plot is water saturation as a function of RH.)

28. p. 6-189, Figure 6.5-8 caption: Change "Constant RH" to "Constant RH = 95%."

29. p. 6-231, last line before Section 6.5.2.7.2: Change "FEP Number 2.1.13.01A" to "FEP Number 2.1.13.01.0A." This same correction is needed in the DIRS entry for the cited reference (DTN: MO0706SPAFEPLA.001 [DIRS 181613]), used in Section 6.5.2.7.1, in the DIRS list for ANL-WIS-PA-000001 REV 03. See Item 32 below for the revised DIRS entry.

30. p. 6-255, 3rd line: Change "3.77×10^{-5} mol m^{-3}" (molar density of ideal gas) to "3.77×10^{-5} mol cm^{-3}."

31. p. 6-255, 2nd paragraph (starting with "The maximum diffusion"): Change "1196 m^2 (from Table 6.3-11)" to "1195 m^2 (from Table 6.3-10)." (Note: 2 errors corrected.)

32. p. 6-304, 1st full paragraph (starting with "The drip shield"), 4th line: Change "FEP Number 2.1.08.11.0A" to "FEP Number 2.1.08.14.0A." This same correction is needed in the DIRS entry for the cited reference (DTN: MO0706SPAFEPLA.001 [DIRS 181613]), used in Section 6.7, in the DIRS list for ANL-WIS-PA-000001 REV 03. The DIRS entries for DTN: MO0706SPAFEPLA.001 [DIRS 181613] are revised as follows:

DIRS entries for DTN: MO0706SPAFEPLA.001 [DIRS 181613] for ANL-WIS-PA-000001 REV 03

FEP Number 2.1.13.01A	Section 6.5.2.7.1	Radiolysis is screened out.	Indirect Input	N/A	N/A	N/A
FEP Number 2.1.08.14.0A	Sections 6.3.3.2.5 and 6.3.3.3	Dripping onto the waste package from condensation on the underside of the drip shield is screened out.	Indirect Input	N/A	N/A	N/A
FEP Number 2.1.08.11.0A	Section 6.7	Condensation on the underside of the drip shield screened out.	Indirect Input	N/A	N/A	N/A

Revised DIRS entries for DTN: MO0706SPAFEPLA.001 [DIRS 181613] for ANL-WIS-PA-000001 REV 03 ERD 02

FEP Number 2.1.13.01.0A	Section 6.5.2.7.1	Radiolysis is screened out.	Indirect Input	N/A	N/A	N/A
FEP Number 2.1.08.14.0A	Sections 6.3.3.2.5, 6.3.3.3, and 6.7	Dripping onto the waste package from condensation on the underside of the drip shield is screened out.	Indirect Input	N/A	N/A	N/A
~~FEP Number 2.1.08.11.0A~~	~~Section 6.7~~	~~Condensation on the underside of the drip shield screened out.~~	~~Indirect Input~~	~~N/A~~	~~N/A~~	~~N/A~~

33. p. 6-304, 2nd full paragraph (starting with "The waste package"), 10th line: Change "6.3.3.3" to "6.3.3.2.5."

34. p. 6-224, 3rd definition following Equation 6.5.2.5-22, for "effective diffusive conductance between UZ fracture and matrix cells": Change "$\hat{D}_{ilf}$" to "$\hat{D}_{imf}$." This error was not identified in CR 12867.

35. p. 5-3, 2nd paragraph of *Basis*, 10th line: Change "Since the lifetime of stainless steel components ranges from 49,800 yr to 5.08 × 10^6 yr (as estimated in Section 6.5.2.2.1)" to "Since the lifetime of stainless steel components ranges from 49,800 yr to 2.54 × 10^6 yr (depending on component thickness, as estimated for the inner vessel in Section 6.5.2.2.1)". This error was not identified in CR 12867.

36. p. 6-181, 11th line: Change "For stainless steel, the lifetime ranges from 49,800 yr to 5.08 × 10^6 yr" to "For stainless steel, the lifetime ranges from 49,800 yr to 2.54 × 10^6 yr." This error was not identified in CR 12867.

37. p. 6-181, 11th line: Change "For carbon steel, the lifetime ranges from 118 yr to 1,270 yr" to "For carbon steel, the lifetime ranges from 118 yr to 635 yr." This error was not identified in CR 12867.

38. p. 6-187, last line, and p. 6-188, 1st line: Change "In this example, stainless steel has a lifetime of 20,800 yr" to "In this example, stainless steel has a lifetime of 20,800 yr, based on the maximum component thickness of 9.525 mm in this domain (Table 6.5-5) and a corrosion rate of 0.229 µm yr^{-1}." This clarification is needed because an earlier statement (clarified in Item #35 above) could have been interpreted to mean that the *minimum* lifetime of stainless steel components is 49,800 yr. This clarification was not identified in CR 12867.

39. p. 6-218, paragraph preceding Eq. 6.5.2.5-1, 2nd line: Change "(Equation 6.5.1.2-48)" to "(Equation 6.5.1.2-47)." This error was not identified in CR 12867.

40. pp. 6-234 – 6-235; several equation number references need to be corrected. These errors were not identified in CR 12867.
    a. p. 6-234, paragraph following Eq. 6.5.2.7.2-8: Change "Equation 6.5.2.7-1" to "Equation 6.5.2.7.2-1" (2 occurrences).
    b. p. 6-234, sentence preceding Eq. 6.5.2.7.2-10: Change "Equation 6.5.2.7-1" to "Equation 6.5.2.7.2-1."
    c. p. 6-235, sentence following Eq. 6.5.2.7.2-14: Change "Equations 6.5.2.7-13 and 6.5.2.7-14" to "Equations 6.5.2.7.2-13 and 6.5.2.7.2-14."
    d. p. 6-235, sentence following Eq. 6.5.2.7.2-14: Change "Equations 6.5.2.7-6 and 6.5.2.7-7" to "Equations 6.5.2.7.2-6 and 6.5.2.7.2-7."

II. CR 12998 Resolution

CR 12998 points out that, in certain modeling cases in the License Application TSPA (TSPA-LA), sorption of radionuclides onto steel corrosion products is over-predicted, with the nonphysical result that the number of moles of radionuclide sorbed exceeds the number of sorption sites available. This occurs in approximately 5% of the simulations in the TSPA-LA (Figure 1), primarily in the Igneous Intrusion Modeling Case for 10,000 years. To resolve CR 12998, the potential impact of the overestimation of sorption on the predicted mean annual dose is evaluated in this ERD by developing a supplemental sorption model that is more accurate under the conditions where the current sorption model breaks down. This supplemental model was tested in a subset of the TSPA-LA analysis to show that an improved sorption model has an insignificant impact on repository performance, i.e., on predicted dose. Since the impact is insignificant, no further action is required to resolve CR 12998. No downstream usage—neither the LA nor other project documents—is impacted.

II.1. Input Data

The models run for this analysis use the same inputs to the TSPA-LA model and are documented in *Total System Performance Assessment Model /Analysis for the License Application* (SNL 2008 [DIRS 183478], Section 4[a]), except where indicated in the Section II.3 below. The source of the regression coefficients for the sorption model in the TSPA-LA is *EBS Radionuclide Transport Abstraction* (SNL 2007 [DIRS 177407], Table 6.5-14).

II.2. Software

The software codes used for this analysis were from the same set of software codes used to run the TSPA-LA Model v5.005 in the TSPA-LA model report (SNL 2008 [DIRS 183478], Section 3[a]). These software codes are qualified and controlled per Lead Laboratory procedure IM-PRO-003, *Software Management*. No software was modified for this analysis. In addition, GoldSim V. 9.60.300 (STN: 10344-9.60-03. [DIRS 184387]) was used to query TSPA baseline simulations and to perform sensitivity analyses with the TSPA model. MView V. 4.0 (STN: 10072-4.0-01 [DIRS 181049] was used for performing regression analyses based on TSPA results. EXDOC_LA V. 2.0 (STN: 11193-2.0-00 [DIRS 182102]) was used to calculate expected values for quantities of interest. PHREEQC V. 2.11.01 (STN: 10068-2.11-01 [DIRS 185868]) was used to perform geochemical modeling and to evaluate the effects of major ions that compete for sorption sites.

Commercial off-the-shelf software, including Microsoft Word and Microsoft Excel, was used in this work. This software is exempt from qualification per Section 2.0 of IM-PRO-003, *Software Management*. Microsoft Word and Microsoft Excel are standard software applications used widely throughout the Yucca Mountain Project (YMP). They provide standard word processing and spreadsheet functions. There are no limitations on the use of the commercial off-the-shelf software used in this document related to their specified functions. No macros or special software routines were used by, or developed for, this software. The work was conducted using Yucca Mountain Project-standard desktop computers.

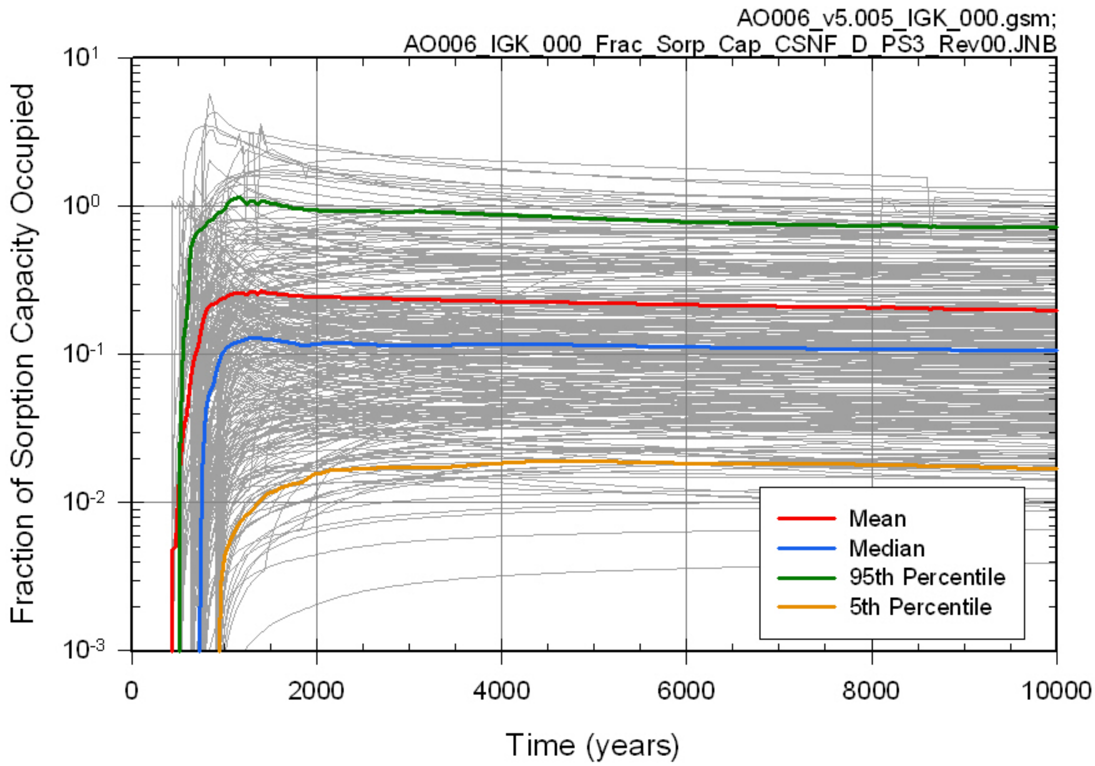
II.3. Analysis

Overestimation of sorption is primarily restricted to the Igneous Intrusion Modeling Case, although it also occurs in rare instances in the Seismic Ground Motion Modeling Case for 10,000 years (Figure 2). In the Igneous Intrusion Modeling Case for 10,000 years, instantaneous degradation of the CSNF waste form following the igneous intrusive event, coupled with higher CO_2 partial pressures (P_{CO_2}) (sometimes exceeding 10^{-2} bar) early in the repository history, leads to high dissolved concentrations and large mass releases by advection and diffusion from Cell 1 (waste form) of the TSPA discretized EBS transport model, at a time when only a small fraction of the steel has corroded and the amount of corrosion products on which sorption can occur is still small. In realizations where the sorption capacity is exceeded, the dissolved concentration of ^{238}U in Cell 1 is typically greater than 10^{-4} mol/L, and the number of sorption sites per liter of water is typically less than 2 mol-sites/L (a value below the 10th percentile of the range, which varies from about 1 to 12 mol-sites/L). Under such conditions, the sorption abstraction calculates low K_d values for uranium (Figure 3). However, the predicted K_d values are not low enough, and sorption is slightly over-predicted. This results from the inherent uncertainty in the multiple regression model used in the TSPA-LA calculations (referred to here as the "base-case K_d model"), which was developed based on the competitive sorption calculations performed using PHREEQC (SNL 2007 [DIRS 177407], Section 6.5.2.4). The coefficient of determination (R^2) is about 0.95 for the regression model that is used to predict uranium sorption (SNL 2007 [DIRS 177407], Table 6.5-14). However, this regression model is based on a large dataset, consisting of the results of PHREEQC simulations with independent parameters that range over several orders of magnitude. When only those data corresponding to high dissolved uranium concentrations (>10^{-4} mol/L) and low sorption sites per liter of water (< 4 mol-sites/L) are considered, the regression model does not provide a good fit (Figure 4a). By performing a multiple regression on the reduced data set, the predictive capability improves for these conditions (Figure 4b). The new regression calculation is contained in the output DTN: MO0812TSPAOSIA.000, in worksheet "U_regress_High_U" of spreadsheet, *Final_Surf_Complx_Regression.xls*. The new regression equation (referred to as the "adjusted K_d model") has the following form:

$$\log_{10}(U_{CP}) = 0.359 - 0.038\, pCO_2 + 0.006\, (pCO_2)^2 + 1.00 \log_{10}(spl) - 0.012 \log_{10}(U) - 0.007\, [\log_{10}(U)]^2, \qquad \text{(Eq. 1)}$$

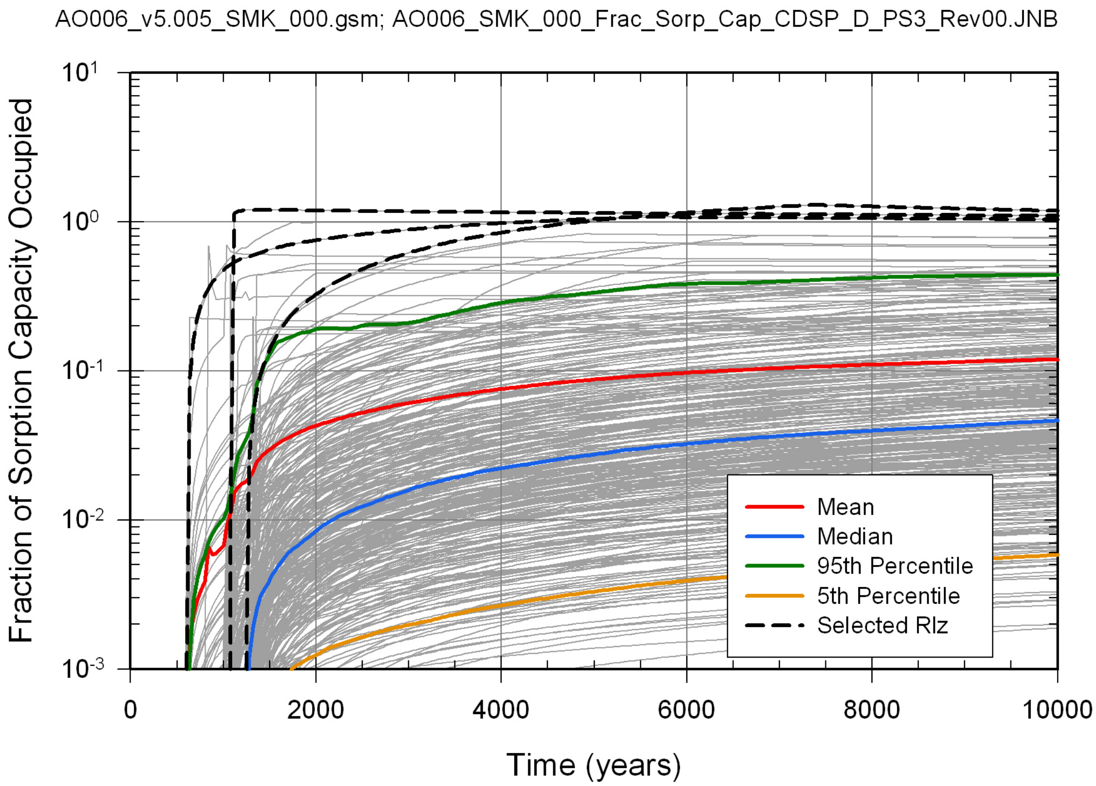
where U_{CP} is the amount of uranium sorbed onto corrosion products in units of sorbed moles per liter of water, U is the dissolved uranium concentration in discretized EBS transport model Cell 2 (waste package corrosion products) in mol/L, spl is the concentration of sorption sites in units of mol-sites/L, and pCO_2 is the negative base-10 log of P_{CO_2}, with P_{CO_2} in units of bar.

Applying Equation 1 (the adjusted K_d model) under the applicable sets of conditions results in lower K_d values for uranium. When the adjusted K_d model is used to recalculate model results for those realizations where sorption capacity was originally exceeded appreciably (by a factor of 2 to 3), the fraction of the sorption capacity that is filled, following an initial pulse, rapidly returns to a value near 1.0 (Figure 5). The Igneous Intrusion Modeling Case for 10,000 years was rerun implementing the adjusted K_d model when the dissolved uranium concentration exceeded 10^{-4} mol/L and concentration of sorption sites was less than 4 mol-sites/L, and the mean annual dose was compared with TSPA-LA results to investigate the effect of using the adjusted K_d model. As shown in Figure 6, the mean annual dose remains largely unchanged. The maximum mean dose increase using the adjusted K_d model was about 0.2% over the TSPA-LA results, indicating that the small number of realizations where the sorption capacity is exceeded does not impact the mean dose. This demonstration that the overestimation of sorption in the TSPA-LA does not significantly impact repository performance resolves CR 12998, and no further action is required.



Output DTN: MO0812TSPAOSIA.000, file MO0812TSPAOSIA_000.zip

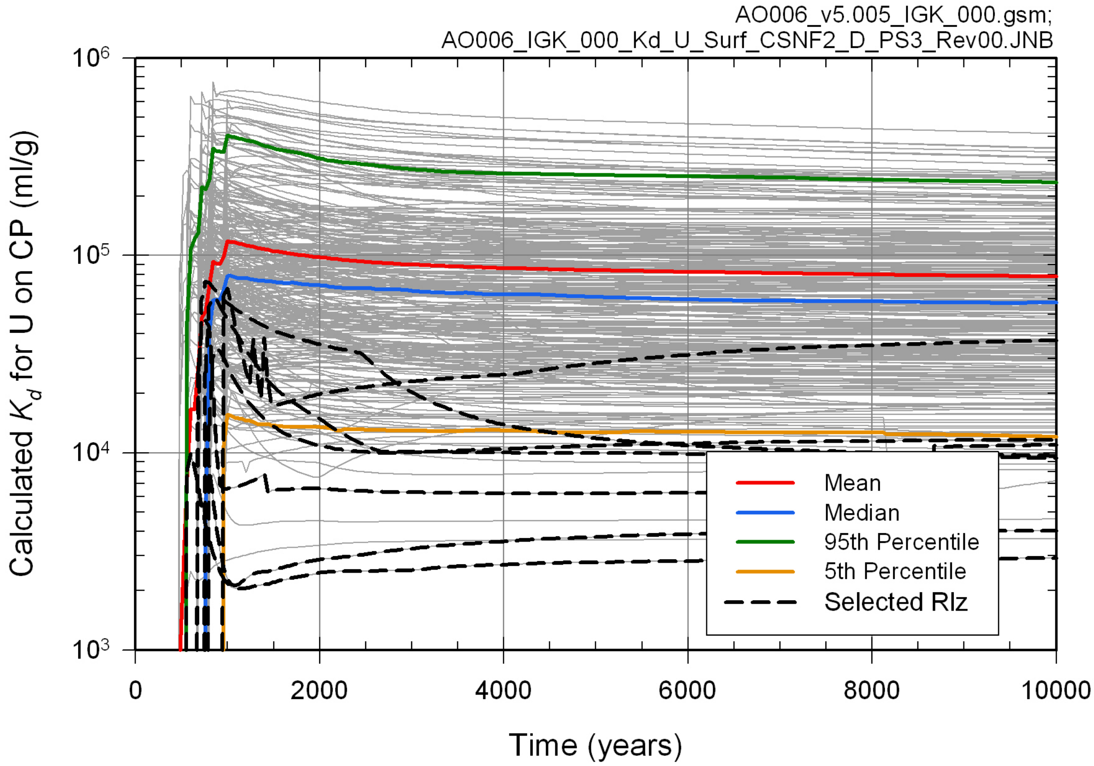
Figure 1. Fraction of Sorption Capacity Occupied for All 300 Realizations in CSNF Waste Packages in Percolation Subregion 3 Dripping Environments after an Igneous Intrusion at 100 Years



Note: Selected realizations (Rlz) indicate instances where sorption is overestimated.

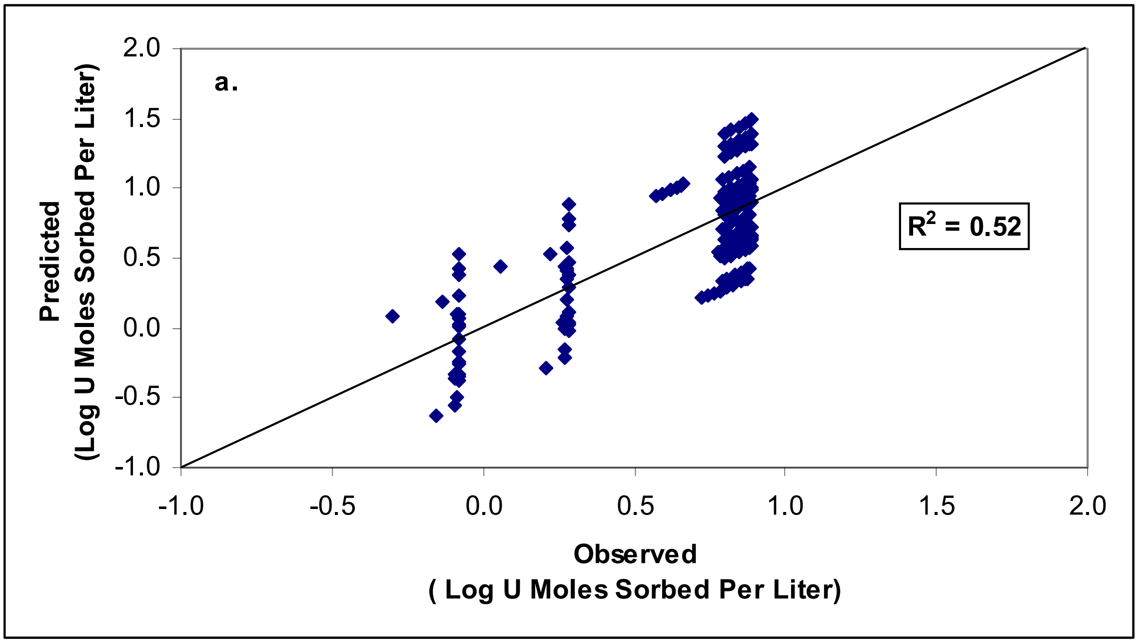
Output DTN: MO0812TSPAOSIA.000, file MO0812TSPAOSIA_000.zip

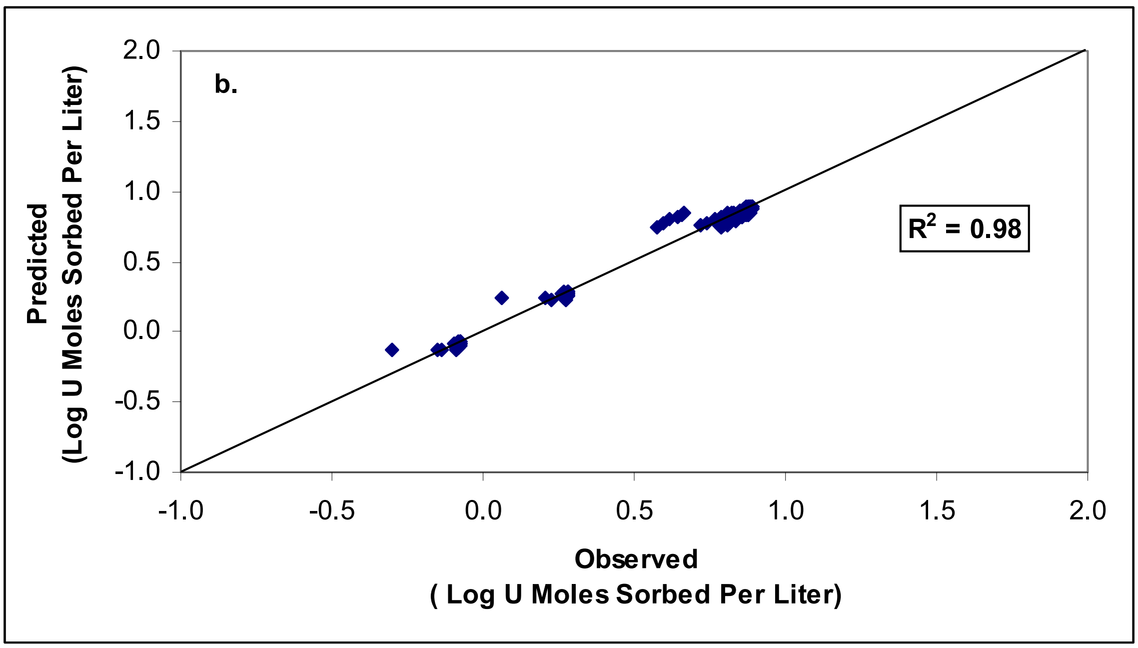
Figure 2. Fraction of Sorption Capacity Occupied for 300 Realizations in Damaged CDSP Waste Packages under Percolation Subregion 3 Dripping Environments after a Seismic Ground Motion Event at 200 Years.



Note: Selected realizations (Rlz) are those instances where sorption is overestimated.
Output DTN: MO0812TSPAOSIA.000, file MO0812TSPAOSIA_000.zip

Figure 3. Calculated K_d for Uranium on the Stationary Corrosion Products in CSNF Waste Packages in Percolation Subregion 3 Dripping Environments after an Igneous Intrusion at 100 Years

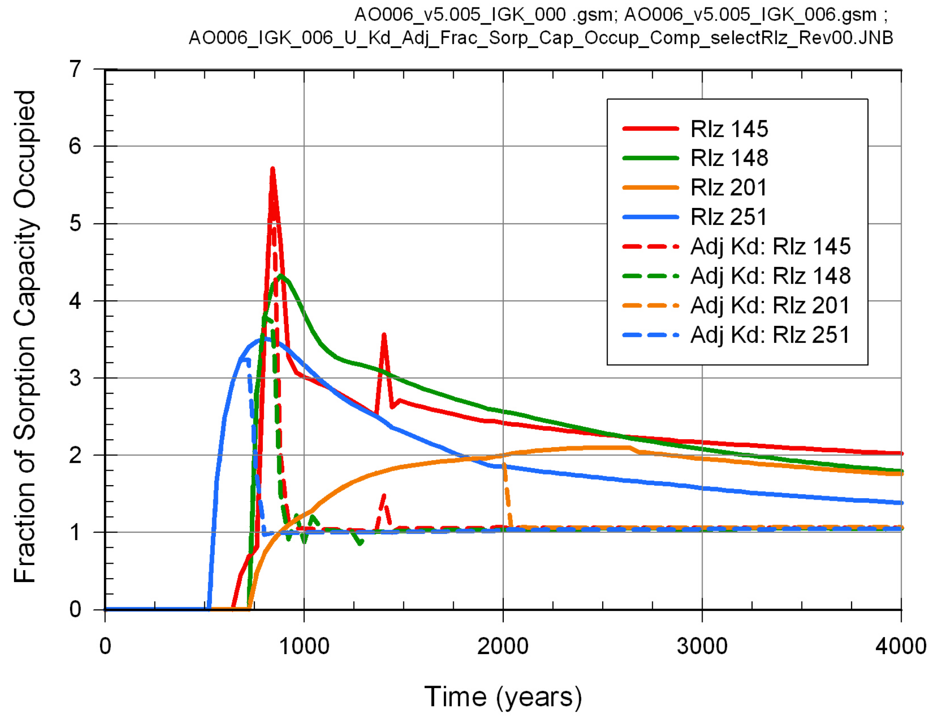




NOTE: The only data sets included are those where dissolved uranium concentration is greater than 10^{-4} mol/L and the sorption sites are less than 4 mol-sites/L.

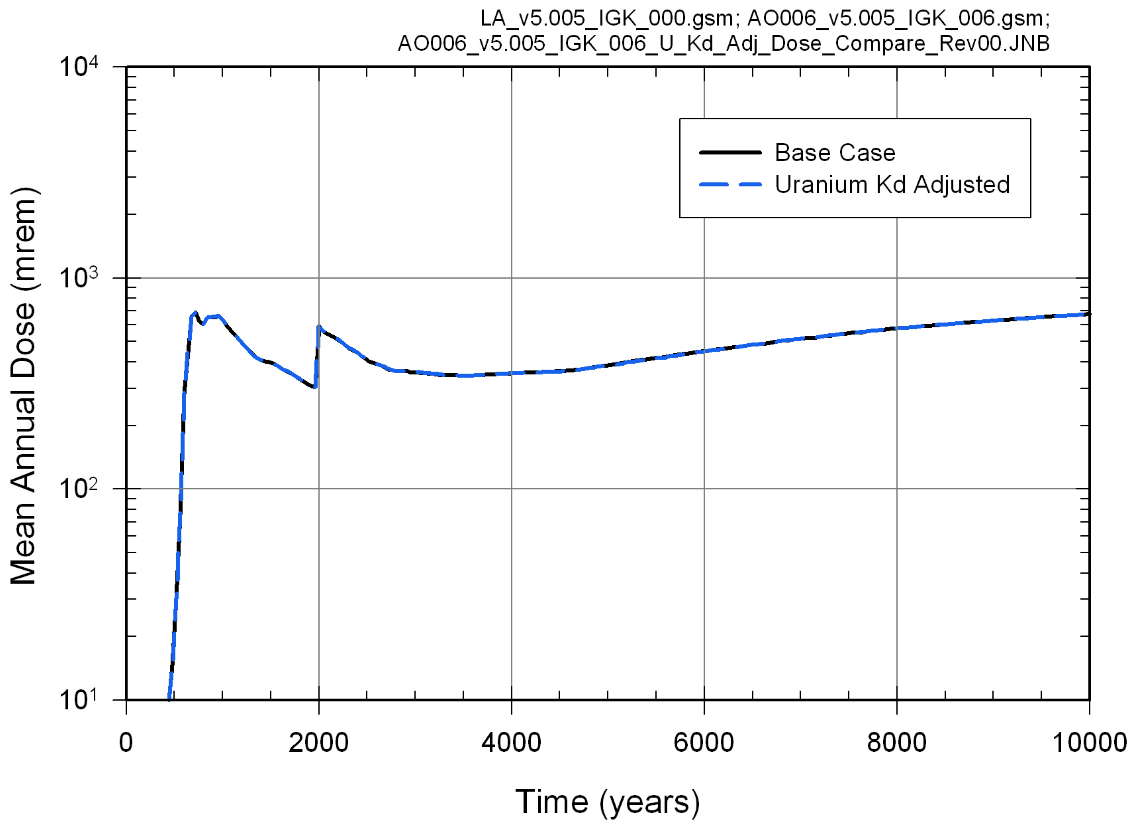
Output DTN: MO0812TSPAOSIA.000, worksheets 'U_data_High_U' and 'U_regress_High_U' in spreadsheet *Final_Surf_Complx_Regression.xls*

Figure 4. Comparison of Predictive Capability of Uranium Sorption (log of moles sorbed per liter of water) Using (a) Base-Case K_d Model and (b) Adjusted K_d Model



Output DTN: MO0812TSPAOSIA.000, file MO0812TSPAOSIA_000.zip

Figure 5. Comparison of Fraction of Sorption Capacity Occupied for Selected Realizations (Rlz) Using Base-Case K_d Model and Adjusted K_d Model for Igneous Intrusion Modeling Case for 10,000 Years for CSNF Waste Packages in Percolation Subregion 3 Seep Environment



Output DTN: MO0812TSPAOSIA.000, file MO0812TSPAOSIA_000.zip

Figure 6. Comparison of Mean Annual Dose Using Base-Case K_d Model and Adjusted K_d Model for Sorption of Uranium on the Corrosion Products for Igneous Intrusion Modeling Case for 10,000 Years

III. CR 13093 Resolution

CR 13093 is resolved by correcting references to design TDIPs in Table 4.1-20, Section 6.5.2.3, and Appendix I of ANL-WIS-PA-000001 REV 03. The following changes are made (see DIRS changes at the end of this list):

1. Table 4.1-20, p. 4-46: For Model Input "Maximum depth of invert," change the Value from "4 ft. 4 in." to "52 in.," and change the Source from "SNL 2007 [DIRS 179354], Table 4-1, Parameter Number 01-10" to "SNL 2007 [DIRS 179354], Figure 4-1."

2. p. 6-190, Section 6.5.2.3, 1st paragraph, lines 3-4: Change "maximum invert thickness of $t_{I,max}$ = 4 ft 4 in. = 1.321 m (SNL 2007 [DIRS 179354], Table 4-1, Parameter Number 01-10)" to "maximum invert thickness of $t_{I,max}$ = 52 in. = 1.321 m (SNL 2007 [DIRS 179354], Figure 4-1)." This change was not specified in CR 13093, but is made to be consistent with the change described in the preceding item.

3. Appendix I, p. I-1, Section I.1, 1st paragraph, lines 7-9: Change "The domain width is 40.5 m, which is half the distance between centers of waste emplacement drifts (SNL 2007 [DIRS 179466], Table 4-1, Parameter No. 01-04)" to "The domain width is 40.5 m, which is half the distance between centers of waste emplacement drifts (SNL 2007 [DIRS 179466], Table 4-1, Parameter No. 01-13)." This error was not listed in CR 13093, but was identified when the DIRS was inspected in responding to this CR.

4. Appendix I, p. I-3, last paragraph, lines 6-7: Change "The drift diameter is 5.5 m (SNL 2007 [DIRS 179466], Table 4-1, Parameter No. 01-04)" to "The drift diameter is 5.5 m (SNL 2007 [DIRS 179466], Table 4-1, Parameter No. 01-10)."

5. Appendix I, p. I-3, last paragraph, lines 11-14: Change "The current invert design calls for a maximum depth of 1.32 m (4 ft 4 in.) … (SNL 2007 [DIRS 179354], Table 4-1, Parameter No. 01-13A)" to "The current invert design calls for a maximum depth of 1.32 m (52 in.) … (SNL 2007 [DIRS 179354], Figure 4-1)." In addition to this change in Appendix I text, this input data reference in Appendix I should be included in the DIRS for ANL-WIS-PA-000001 REV 03; this omission was not listed in CR 13093, but was identified when the DIRS was inspected in response to this CR.

The DIRS entries for ANL-WIS-PA-000001 REV 03 are revised as follows to resolve CR 13093. Changes to the DIRS noted below are marked up on the point-in-time DIRS report, and the revised DIRS report is processed in accordance with SCI-PRO-004, *Managing Technical Product Inputs*; the marked-up pages from the DIRS report are appended to this ERD (new DIRS entries are not shown in the appended DIRS mark-up but are listed in Attachment I).

DIRS entry for SNL 2007 [DIRS 179354] for ANL-WIS-PA-000001 REV 03

Table 4-1, Parameter Number 01-10	Table 4.1-20; Section 6.5.2.3	Maximum depth of invert	Indirect Input	N/A	N/A	TBV-8613 Resolved

Revised DIRS entry for SNL 2007 [DIRS 179354] for ANL-WIS-PA-000001 REV 03 ERD 02

Figure 4-1	Table 4.1-20; Section 6.5.2.3; Appendix I.1	Maximum depth of invert	Indirect Input	N/A	N/A	TBV-8613 Resolved

DIRS entry for SNL 2007 [DIRS 179466] for ANL-WIS-PA-000001 REV 03

Table 4-1; Parameter 01-04	Appendix I.1	Development of the grid of the two-dimensional symmetry model	Indirect Input	N/A	N/A	TBV-8614 Resolved

Revised and new DIRS entries for SNL 2007 [DIRS 179466] for ANL-WIS-PA-000001 REV 03 ERD 02

Table 4-1; Parameter 01-13	Appendix I.1	Distance between centers of waste emplacement drifts	Indirect Input	N/A	N/A	TBV-8614 Resolved
Table 4-1; Parameter 01-10	Appendix I.1	Drift diameter	Indirect Input	N/A	N/A	N/A

None of the changes in response to CR 13093 impacts the conclusions of ANL-WIS-PA-000001 REV 03, and no downstream usage—neither the LA nor other project documents—is impacted.

IV. CR 10788 Resolution

CR 10788 addresses a procedural non-compliance regarding qualification of external source data used as direct input. A review of ANL-WIS-PA-000001 REV 03 revealed that most of the information required for the qualification of external data was presented in the document, but some of the documentation requirements of SCI-PRO-001, *Qualification of Unqualified Data*, were omitted. The documentation deficiency is resolved by Table 1, which contains the external sources listed in Section 4 of ANL-WIS-PA-000001 REV 03 and used as direct input. The table contains the method used for qualification, the rationale for choosing that method, the qualification attributes, and the location within the document where the qualification information is presented.

For most of the inputs listed in Table 1, attribute 10, corroboration with other data, is listed as one of the attributes used for demonstrating qualification for intended use. For site density (goethite and HFO), specific surface area (goethite, HFO, and CSNF-related oxides), and water vapor adsorption isotherm (iron oxides and CSNF-related oxides), the input values coming from different sources were combined to provide ranges or probability distributions for use in the analysis. The last column of Table 1 indicates the location within the document where the data were compiled and distributions were developed. All of the values are considered qualified because they are corroborated by the other values in each data set. All inputs are judged to be qualified for intended use within ANL-WIS-PA-000001 REV 03, in accordance with SCI-PRO-006, *Models*, Section 6.2.1.L(3), based on the qualification attributes listed in Table 1.

For one of the direct inputs listed in Table 1, Ebert et al. (1991 [DIRS 111028]), the qualification documentation within Section 4 is revised so that the data is qualified in accordance with SCI-PRO-001, as required by SCI-PRO-006, Section 6.2.1.L(1), which applies to data developed by YMP participants. The first paragraph of p. 4–13 is revised as follows, with new text underlined:

> **Water vapor isotherm for HLW glass**—The Frenkel-Halsey-Hill (FHH) adsorption isotherm parameters *k* and *s* for HLW glass are provided by Ebert et al. (1991 [DIRS 111028], p. 134, Figure 1b). The parameters were determined by curve-fitting data representing the number of water monolayers versus relative humidity for HLW glass. Ebert et al. (1991 [DIRS 111028], p. 134, Figure 1a) also present an isotherm for natural

obsidian that shows lower values of adsorption than for the HLW glass. The natural obsidian isotherm is corroborated by a nearly identical isotherm for silica and quartz presented in Hagymassy et al. (1968 [DIRS 111034], p. 489). Corroboration of the natural obsidian isotherm by Hagymassy et al. (1968 [DIRS 111034]) gives confidence that the isotherm measured by Ebert for nuclear waste glass is also accurate. Ebert has studied HLW glass at Argonne National Laboratory for many years and has published many articles in peer-reviewed journals. These data were developed by Ebert while supporting the project and are reported in *Defense HLW Glass Degradation Model* (BSC 2004 [DIRS 169988], Section 6.5.3.1). The values of isotherm parameters *k* and *s* are qualified in accordance with SCI-PRO-001. The data qualification team consisted of James Schreiber (B.S. and M.S. Chemical Engineering, with twenty years experience in nuclear waste management) and Susan LeStrange (M.S. Chemical Engineering, Ph.D. Agricultural Engineering, with expertise in geochemistry and chemical transport). The data qualification team concluded that the data are corroborated by Hagymassy et al. (1968 [DIRS 111034]). Therefore, the data are qualified and appropriate for use in the RTA.

The following new reference is added to Section 9.1

111034 Hagymassy, J., Jr.; Brunauer, S.; and Mikhail, R.Sh. 1969. "Pore Structure Analysis by Water Vapour Absorption. Part 1. T-Curves for Water Vapour." *Journal of Colloid and Interface Science, 29,* (3), 485-491. New York, New York: Academic Press. TIC: 246076.

In Table 6.5–9, change the value of "FHH adsorption isotherm parameter *k* for HLW glass", from "13.2" to "3.2".

The DIRS entries for "Input usage" for some of the inputs in Section 4 were incorrectly classified as "Indirect Input" rather than "Direct Input". In addition, the DIRS entries for "Input Category" for some inputs were incorrectly labeled as "Data" rather than "Established Fact". The changes to the DIRS are provided in Table 2. Table 2 also lists various other changes to the DIRS, including further changes prompted by the Indirect/Direct reclassification described in this section as well as related miscellaneous clarifications and corrections that were made in response to CR 10788.

None of the changes in response to CR 10788 impacts the conclusions of ANL-WIS-PA-000001 REV 03. As a result, neither the LA nor other project documents is impacted.

Table 1. Data Qualification for External Source Data Qualified for Intended Use in Document ANL-WIS-PA-000001 REV 03

Input	Source	Description	Method[1] (Rationale)[2]	Attribute[3]	Locations within AMR Where Data Are Listed and Where Qualification Is Documented or Corroboration Is Demonstrated
McCafferty and Zettlemoyer 1970 [DIRS 154382]	p. 454	Water molecule cross-sectional area, A_w	5 (a,b)	1, 3, 7, 10	Table 4.1-11, p. 4-12
	Figure 3	Water Vapor Adsorption Isotherms for α-Fe_2O_3	5 (a)	3, 10	Table 4.1-19, p. 4-33, Section 6.3.4.3.2, p. 6-72, Figure 6.3-34, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Corrosion Products Composite Isotherm 7-19-2007.xls*
Towe and Bradley 1967 [DIRS 155334]	p. 386	Density of HFO	5 (b)	3, 7, 10	Table 4.1-11, pp. 4-15 and 4-16
Ebert, Hoburg, and Bates 1991 [DIRS 111028]	p. 134, Figure 1b	Parameters *k* and *s* in FHH water vapor adsorption isotherm for HLW glass	5 (c)	1, 3, 7, 10	Table 4.1-11, p. 4-13, Section IV of this ERD
Rodda et al. 1996 [DIRS 173710]	Table 1, Table 5	Goethite site density	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Tables 6.3-4 and 6.3-5
	p. 365	Goethite specific surface area	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Section 6.3.4.3.3, Appendix K, Figure K-5, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Goethite specific surface area 7-12-2007.xls*
Hiemstra and Van Riemsdijk 1996 [DIRS 173023]	p. 498	Goethite site density	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Tables 6.3-4 and 6.3-5
Villalobos et al. 2003 [DIRS 173017]	Table 2	Goethite site density	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Tables 6.3-4 and 6.3-5
	Table 2	Goethite specific surface area	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Section 6.3.4.3.3, Appendix K, Figure K-5, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Goethite specific surface area 7-12-2007.xls*
Trivedi et al. 2001 [DIRS 173021]	Table 3	Goethite site density	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Tables 6.3-4 and 6.3-5
	Table 3	Goethite specific surface area	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Section 6.3.4.3.3, Appendix K, Figure K-5, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Goethite specific surface area 7-12-2007.xls*

Table 1. Data Qualification for External Source Data Qualified for Intended Use in Document ANL-WIS-PA-000001 REV 03 (Continued)

Input	Source	Description	Method[1] (Rationale)[2]	Attribute[3]	Locations within AMR Where Data Are Listed and Where Qualification Is Documented or Corroboration Is Demonstrated
Naveau et al. 2005 [DIRS 173018]	p. 6	Goethite site density	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Tables 6.3-4 and 6.3-5
	p. 6	Goethite specific surface area	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Section 6.3.4.3.3, Appendix K, Figure K-5, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Goethite specific surface area 7-12-2007.xls*
Coughlin and Stone 1995 [DIRS 173030]	Table 1	Goethite site density	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Tables 6.3-4 and 6.3-5
	Table 1	Goethite specific surface area	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Section 6.3.4.3.3, Appendix K, Figure K-5, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Goethite specific surface area 7-12-2007.xls*
Grossl et al. 1997 [DIRS 173032]	p. 322	Goethite site density	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Tables 6.3-4 and 6.3-5
	p. 322	Goethite specific surface area	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Section 6.3.4.3.3, Appendix K, Figure K-5, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Goethite specific surface area 7-12-2007.xls*
Fendorf et al. 1996 [DIRS 173034]	p. 100	Goethite site density	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Tables 6.3-4 and 6.3-5
	p. 100	Goethite specific surface area	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Section 6.3.4.3.3, Appendix K, Figure K-5, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Goethite specific surface area 7-12-2007.xls*
Duc et al. 2003 [DIRS 173019]	Table 2	Goethite site density	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Tables 6.3-4 and 6.3-5
	Table 1	Goethite specific surface area	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Section 6.3.4.3.3, Appendix K, Figure K-5, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Goethite specific surface area 7-12-2007.xls*
Pivovarov 1997 [DIRS 173714]	Table 1	Goethite site density	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Tables 6.3-4 and 6.3-5

Table 1. Data Qualification for External Source Data Qualified for Intended Use in Document ANL-WIS-PA-000001 REV 03 (Continued)

Input	Source	Description	Method[1] (Rationale)[2]	Attribute[3]	Locations within AMR Where Data Are Listed and Where Qualification Is Documented or Corroboration Is Demonstrated
Gräfe et al. 2004 [DIRS 173751]	p. 6561	Goethite site density	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Tables 6.3-4 and 6.3-5
	p. 6562	Goethite specific surface area	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Section 6.3.4.3.3, Appendix K, Figure K-5, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Goethite specific surface area 7-12-2007.xls*
Missana et al. 2003 [DIRS 173759]	p. 296	Goethite site density	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Tables 6.3-4 and 6.3-5
	Table 3	Goethite specific surface area	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Section 6.3.4.3.3, Appendix K, Figure K-5, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Goethite specific surface area 7-12-2007.xls*
Lützenkirchen et al. 2002 [DIRS 173757]	p. 3394, Table 1	Goethite site density	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Tables 6.3-4 and 6.3-5
Müller and Sigg 1992 [DIRS 173760]	p. 519	Goethite site density	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Tables 6.3-4 and 6.3-5
	p. 519	Goethite specific surface area	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Section 6.3.4.3.3, Appendix K, Figure K-5, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Goethite specific surface area 7-12-2007.xls*
Randall et al. 1999 [DIRS 173709]	Table 1	Goethite site density	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Tables 6.3-4 and 6.3-5
	Table 1	Goethite specific surface area	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Section 6.3.4.3.3, Appendix K, Figure K-5, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Goethite specific surface area 7-12-2007.xls*
Felmy and Rustad 1998 [DIRS 173708]	p. 26	Goethite site density	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Tables 6.3-4 and 6.3-5
	p. 27	Goethite specific surface area	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Section 6.3.4.3.3, Appendix K, Figure K-5, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Goethite specific surface area 7-12-2007.xls*

Table 1. Data Qualification for External Source Data Qualified for Intended Use in Document ANL-WIS-PA-000001 REV 03 (Continued)

Input	Source	Description	Method[1] (Rationale)[2]	Attribute[3]	Locations within AMR Where Data Are Listed and Where Qualification Is Documented or Corroboration Is Demonstrated
Hongshao and Stanforth 2001 [DIRS 173754]	p. 4754	Goethite site density	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Tables 6.3-4 and 6.3-5
	p. 4754	Goethite specific surface area	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Section 6.3.4.3.3, Appendix K, Figure K-5, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Goethite specific surface area 7-12-2007.xls*
Buerge-Weirich et al. 2002 [DIRS 173752]	p. 329	Goethite site density	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Tables 6.3-4 and 6.3-5
	p. 329	Goethite specific surface area	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Section 6.3.4.3.3, Appendix K, Figure K-5, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Goethite specific surface area 7-12-2007.xls*
Boily et al. 2001 [DIRS 173707]	Table 3	Goethite site density	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Tables 6.3-4 and 6.3-5
	Table 3	Goethite specific surface area	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Section 6.3.4.3.3, Appendix K, Figure K-5, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Goethite specific surface area 7-12-2007.xls*
Gao and Mucci 2001 [DIRS 173750]	p. 2364	Goethite site density	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Tables 6.3-4 and 6.3-5
	p. 2362	Goethite specific surface area	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Section 6.3.4.3.3, Appendix K, Figure K-5, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Goethite specific surface area 7-12-2007.xls*
Robertson and Leckie 1997 [DIRS 173763]	Table 4	Goethite site density	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Tables 6.3-4 and 6.3-5
	Table 3	Goethite specific surface area	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Section 6.3.4.3.3, Appendix K, Figure K-5, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Goethite specific surface area 7-12-2007.xls*

Table 1. Data Qualification for External Source Data Qualified for Intended Use in Document ANL-WIS-PA-000001 REV 03 (Continued)

Input	Source	Description	Method[1] (Rationale)[2]	Attribute[3]	Locations within AMR Where Data Are Listed and Where Qualification Is Documented or Corroboration Is Demonstrated
Lövgren et al. 1990 [DIRS 173771]	p. 1303	Goethite site density	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Tables 6.3-4 and 6.3-5
	p. 1301	Goethite specific surface area	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Section 6.3.4.3.3, Appendix K, Figure K-5, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Goethite specific surface area 7-12-2007.xls*
Machesky et al. 1991 [DIRS 173758]	p. 771	Goethite site density	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Tables 6.3-4 and 6.3-5
	p. 770	Goethite specific surface area	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Section 6.3.4.3.3, Appendix K, Figure K-5, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Goethite specific surface area 7-12-2007.xls*
Hayes and Leckie 1987 [DIRS 173817]	Table II	Goethite site density	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Tables 6.3-4 and 6.3-5
	Table II	Goethite specific surface area	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Section 6.3.4.3.3, Appendix K, Figure K-5, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Goethite specific surface area 7-12-2007.xls*
van Geen et al. 1994 [DIRS 144702]	Table 1	Goethite site density	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Tables 6.3-4 and 6.3-5
	Table 1	Goethite specific surface area	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Section 6.3.4.3.3, Appendix K, Figure K-5, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Goethite specific surface area 7-12-2007.xls*
Persson et al. 1998 [DIRS 173762]	p. 261, Table 1	Goethite site density	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Tables 6.3-4 and 6.3-5
	p. 261, Table 1	Goethite specific surface area	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Section 6.3.4.3.3, Appendix K, Figure K-5, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Goethite specific surface area 7-12-2007.xls*

Table 1. Data Qualification for External Source Data Qualified for Intended Use in Document ANL-WIS-PA-000001 REV 03 (Continued)

Input	Source	Description	Method[1] (Rationale)[2]	Attribute[3]	Locations within AMR Where Data Are Listed and Where Qualification Is Documented or Corroboration Is Demonstrated
Davis and Upadhyaya 1996 [DIRS 173743]	p. 1895	Goethite site density	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Tables 6.3-4 and 6.3-5
	p. 1895	Goethite specific surface area	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Section 6.3.4.3.3, Appendix K, Figure K-5, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Goethite specific surface area 7-12-2007.xls*
Xue and Traina 1996 [DIRS 173713]	p. 3163	Goethite site density	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Tables 6.3-4 and 6.3-5
	p. 3161	Goethite specific surface area	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Section 6.3.4.3.3, Appendix K, Figure K-5, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Goethite specific surface area 7-12-2007.xls*
Hansmann and Anderson 1985 [DIRS 173742]	p. 547	Goethite site density	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Tables 6.3-4 and 6.3-5
	p. 546	Goethite specific surface area	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Section 6.3.4.3.3, Appendix K, Figure K-5, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Goethite specific surface area 7-12-2007.xls*
Gabriel et al. 1998 [DIRS 130407]	pp. 124, 126	Goethite site density	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Tables 6.3-4 and 6.3-5
	p. 123	Goethite specific surface area	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Section 6.3.4.3.3, Appendix K, Figure K-5, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Goethite specific surface area 7-12-2007.xls*
Christophi and Axe 2000 [DIRS 173020]	Table 1	Goethite specific surface area	5 (a)	7, 10	Table 4.1-12, pp. 4-13 through 4-15, Section 6.3.4.3.3, Appendix K, Figure K-5, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Goethite specific surface area 7-12-2007.xls*
Cornejo et al. 1984 [DIRS 178660]	Table 1	HFO specific surface area	5 (a)	2, 10	Table 4.1-14, p. 4-16, Section 6.3.4.3.3, Appendix K, Figure K-4, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *HFO_Sp_Surf_Area_Analysis 7-12-2007.xls*

Table 1. Data Qualification for External Source Data Qualified for Intended Use in Document ANL-WIS-PA-000001 REV 03 (Continued)

Input	Source	Description	Method[1] (Rationale)[2]	Attribute[3]	Locations within AMR Where Data Are Listed and Where Qualification Is Documented or Corroboration Is Demonstrated
Cornejo 1987 [DIRS 178659]	Table 1	HFO specific surface area	5 (a)	2, 10	Table 4.1-14, p. 4-16, Section 6.3.4.3.3, Appendix K, Figure K-4, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *HFO_Sp_Surf_Area_Analysis 7-12-2007.xls*
Schwertmann et al. 2004 [DIRS 178734]	Table 1	HFO specific surface area	5 (a)	2, 10	Table 4.1-14, p. 4-16, Section 6.3.4.3.3, Appendix K, Figure K-4, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *HFO_Sp_Surf_Area_Analysis 7-12-2007.xls*
Mitov et al. 2002 [DIRS 178686]	Table 5	HFO specific surface area	5 (a)	2, 10	Table 4.1-14, p. 4-16, Section 6.3.4.3.3, Appendix K, Figure K-4, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *HFO_Sp_Surf_Area_Analysis 7-12-2007.xls*
Clausen and Fabricius 2000 [DIRS 178655]	Table 2	HFO specific surface area	5 (a)	2, 10	Table 4.1-14, p. 4-16, Section 6.3.4.3.3, Appendix K, Figure K-4, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *HFO_Sp_Surf_Area_Analysis 7-12-2007.xls*
O'Reilly and Hochella 2003 [DIRS 178704]	Table 1	HFO specific surface area	5 (a)	2, 10	Table 4.1-14, p. 4-16, Section 6.3.4.3.3, Appendix K, Figure K-4, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *HFO_Sp_Surf_Area_Analysis 7-12-2007.xls*
Sani et al. 2004 [DIRS 178727]	p. 2640	HFO specific surface area	5 (a)	2, 10	Table 4.1-14, p. 4-16, Section 6.3.4.3.3, Appendix K, Figure K-4, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *HFO_Sp_Surf_Area_Analysis 7-12-2007.xls*
Hofmann et al. 2004 [DIRS 173783]	Table 1	HFO specific surface area	5 (a)	2, 10	Tables 4.1-14 and 4.1-19, p. 4-16, Section 6.3.4.3.3, Appendix K, Figure K-4, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *HFO_Sp_Surf_Area_Analysis 7-12-2007.xls*
	Figure 8	Water Vapor Adsorption Isotherms for HFO	5 (a)	3, 10	Table 4.1-19, p. 4-33, Section 6.3.4.3.2, p. 6-72, Figure 6.3-34, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Corrosion Products Composite Isotherm 7-19-2007.xls*
Sauvé et al. 2000 [DIRS 178732]	Table 1	HFO specific surface area	5 (a)	2, 10	Table 4.1-14, p. 4-16, Section 6.3.4.3.3, Appendix K, Figure K-4, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *HFO_Sp_Surf_Area_Analysis 7-12-2007.xls*
Weidler 1997 [DIRS 178741]	Table 1	HFO specific surface area	5 (a)	2, 10	Table 4.1-14, p. 4-16, Section 6.3.4.3.3, Appendix K, Figure K-4, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *HFO_Sp_Surf_Area_Analysis 7-12-2007.xls*

Table 1. Data Qualification for External Source Data Qualified for Intended Use in Document ANL-WIS-PA-000001 REV 03 (Continued)

Input	Source	Description	Method[1] (Rationale)[2]	Attribute[3]	Locations within AMR Where Data Are Listed and Where Qualification Is Documented or Corroboration Is Demonstrated
Guzman et al. 1994 [DIRS 178669]	Table 1	HFO specific surface area	5 (a)	2, 10	Table 4.1-14, p. 4-16, Section 6.3.4.3.3, Appendix K, Figure K-4, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *HFO_Sp_Surf_Area_Analysis 7-12-2007.xls*
Larsen and Postma 2001 [DIRS 178683]	Table 2	HFO specific surface area	5 (a)	2, 10	Table 4.1-14, p. 4-16, Section 6.3.4.3.3, Appendix K, Figure K-4, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *HFO_Sp_Surf_Area_Analysis 7-12-2007.xls*
Leone et al. 2001 [DIRS 178684]	p. 1317	HFO specific surface area	5 (a)	2, 10	Table 4.1-14, p. 4-16, Section 6.3.4.3.3, Appendix K, Figure K-4, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *HFO_Sp_Surf_Area_Analysis 7-12-2007.xls*
Davis and Leckie 1978 [DIRS 125591]	p. 95	HFO specific surface area	5 (a)	10	Table 4.1-14, p. 4-16, Section 6.3.4.3.3, Appendix K, Figure K-4, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *HFO_Sp_Surf_Area_Analysis 7-12-2007.xls*
Liaw et al. 1989 [DIRS 178685]	Table 1	HFO specific surface area	5 (a)	2, 10	Table 4.1-14, p. 4-16, Section 6.3.4.3.3, Appendix K, Figure K-4, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *HFO_Sp_Surf_Area_Analysis 7-12-2007.xls*
Crosby et al. 1983 [DIRS 178662]	Table II	HFO specific surface area	5 (a)	2, 10	Table 4.1-14, p. 4-16, Section 6.3.4.3.3, Appendix K, Figure K-4, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *HFO_Sp_Surf_Area_Analysis 7-12-2007.xls*
Axe and Anderson 1995 [DIRS 178654]	p. 159	HFO specific surface area	5 (a)	2, 10	Table 4.1-14, p. 4-16, Section 6.3.4.3.3, Appendix K, Figure K-4, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *HFO_Sp_Surf_Area_Analysis 7-12-2007.xls*
Van der Giessen 1966 [DIRS 178740]	Table 1	HFO specific surface area	5 (a)	2, 10	Table 4.1-14, p. 4-16, Section 6.3.4.3.3, Appendix K, Figure K-4, output DTN: SN0703PAEBSRTA.001, file *HFO_Sp_Surf_Area_Analysis 7-12-2007.xls*
Davies-Colley et al. 1984 [DIRS 178666]	p. 492	HFO specific surface area	5 (a)	2, 10	Table 4.1-14, p. 4-16, Section 6.3.4.3.3, Appendix K, Figure K-4, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *HFO_Sp_Surf_Area_Analysis 7-12-2007.xls*
Tipping 1981 [DIRS 178737]	Table 1	HFO specific surface area	5 (a)	2, 10	Table 4.1-14, p. 4-16, Section 6.3.4.3.3, Appendix K, Figure K-4, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *HFO_Sp_Surf_Area_Analysis 7-12-2007.xls*
Carlson and Schwertmann 1981 [DIRS 142788]	Table 1	HFO specific surface area	5 (a)	2, 10	Table 4.1-14, p. 4-16, Section 6.3.4.3.3, Appendix K, Figure K-4, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *HFO_Sp_Surf_Area_Analysis 7-12-2007.xls*

Table 1. Data Qualification for External Source Data Qualified for Intended Use in Document ANL-WIS-PA-000001 REV 03 (Continued)

Input	Source	Description	Method[1] (Rationale)[2]	Attribute[3]	Locations within AMR Where Data Are Listed and Where Qualification Is Documented or Corroboration Is Demonstrated
Eggleton and Fitzpatrick 1988 [DIRS 173878]	Table 1	HFO specific surface area	5 (a)	2, 10	Table 4.1-14, p. 4-16, Section 6.3.4.3.3, Appendix K, Figure K-4, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *HFO_Sp_Surf_Area_Analysis 7-12-2007.xls*
Conca and Wright 1992 [DIRS 100436]	Figure 2	Diffusion coefficients for granular materials	2 (e)	3, 8, 10	Table 4.1-16, Appendix H
Conca et al. 1993 [DIRS 170709]	Figure 2	Diffusion coefficients for granular materials	2 (e)	3, 8, 10	Table 4.1-16, Appendix H
Turner and Sassman 1996 [DIRS 179618]	Tables 1 and 3	Surface Complexation Constants	5 (a)	3, 10	Table 4.1-17, p. 4-29, Appendix J, Tables J-2 and J-3
Wang et al. 2001 [DIRS 176816]	Tables 3 and 4	Surface Complexation Constants	5 (a)	3, 10	Table 4.1-17, p. 4-29, Appendix J, Tables J-2 and J-3
Pepper et al.2006 [DIRS 179622]	Table 2	Surface Complexation Constants	5 (a)	3, 10	Table 4.1-17, p. 4-29, Appendix J, Tables J-2 and J-3
Cromières et al. 1998 [DIRS 179616]	Table 4	Surface Complexation Constants	5 (a)	3, 10	Table 4.1-17, p. 4-29, Appendix J, Tables J-2 and J-3
Appelo et al. 2002 [DIRS 168168]	Table 2	Surface Complexation Constants	5 (a)	3, 10	Table 4.1-17, p. 4-29, Appendix J, Table J-2
LaVerne and Tandon 2003 [DIRS 178303]	Figure 1	Water Vapor Adsorption Isotherms for UO_2 and CeO_2	5 (a)	3, 10	Table 4.1-18, p. 4-30, Section 6.3.4.6.1, Figure 6.3-42, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *CSNF Isotherm Compilation 7-19-2007.xls*
	p. 13624	Specific surface area for UO_2 and CeO_2	5 (a)	3, 10	Table 4.1-18, p. 4-30, Section 6.3.4.6.1, Table 6.3-12
Gammage et al. 1970 [DIRS 178304]	Figure 2 p. 4277	Water Vapor Adsorption Isotherm for ThO_2 Specific surface area for ThO_2	5 (a)	3, 10	Table 4.1-18, p. 4-30, Section 6.3.4.6.1, Figure 6.3-42, Table 6.3-12, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *CSNF Isotherm Compilation 7-19-2007.xls*
Holmes et al. 1974 [DIRS 154379]	Figure 3	Water Vapor Adsorption Isotherm for ZrO_2	5 (a)	3, 10	Table 4.1-18, p. 4-30, Section 6.3.4.6.1, Figure 6.3-42, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *CSNF Isotherm Compilation 7-19-2007.xls*
	p. 368	Specific surface area for ZrO_2	5 (a)	3, 10	Table 4.1-18, p. 4-30, Section 6.3.4.6.1, Table 6.3-12

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Input	Source	Description	Method[1] (Rationale)[2]	Attribute[3]	Locations within AMR Where Data Are Listed and Where Qualification Is Documented or Corroboration Is Demonstrated
Stakebake 1971 [DIRS 178302]	Figure 8	Water Vapor Adsorption Isotherm for PuO_2	5 (a)	3, 10	Table 4.1-18, p. 4-30, Section 6.3.4.6.1, Figure 6.3-42, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *CSNF Isotherm Compilation 7-19-2007.xls*
	p. 253	Specific surface area for PuO_2	5 (a)	3, 10	Table 4.1-18, p. 4-30, Section 6.3.4.6.1, Table 6.3-12
Stakebake and Dringman 1968 [DIRS 178840]	Figure 3, Figure 4	Water Vapor Adsorption Isotherm for PuO_2	5 (a)	3, 10	Table 4.1-18, p. 4-30, Section 6.3.4.6.1, Figure 6.3-42, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *CSNF Isotherm Compilation 7-19-2007.xls*
	Table 1	Specific surface area for PuO_2	5 (a)	3, 10	Table 4.1-18, p. 4-30, Section 6.3.4.6.1, Table 6.3-12
Paffett et al. 2003 [DIRS 178712]	Figure 8	Water Vapor Adsorption Isotherm for PuO_2	5 (a)	3, 10	Table 4.1-18, p. 4-30, Section 6.3.4.6.1, Figure 6.3-42, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *CSNF Isotherm Compilation 7-19-2007.xls*
	Table 1	Specific surface area for PuO_2	5 (a)	3, 10	Table 4.1-18, p. 4-30, Section 6.3.4.6.1, Table 6.3-12
Kandori and Ishikawa 1991 [DIRS 178680]	Figure 2	Water Vapor Adsorption Isotherm for amorphous ferric oxide hydroxide	5 (a)	3, 10	Table 4.1-19, p. 4-33, Section 6.3.4.3.2, p. 6-72, Figure 6.3-34, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Corrosion Products Composite Isotherm 7-19-2007.xls*
Koch and Møller 1987 [DIRS 173784]	Figures 5 and 6	Water Vapor Adsorption Isotherms for goethite	5 (a)	3, 10	Table 4.1-19, p. 4-33, Section 6.3.4.3.2, p. 6-72, Figure 6.3-34, output DTN: SN0703PAEBSRTA.001, file *Corrosion Products Composite Isotherm 7-19-2007.xls*
	Table 1	Goethite specific surface area	5 (a)	7, 10	Table 4.1-19, pp. 4-13 through 4-15, Section 6.3.4.3.3, Appendix K, Figure K-5, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Goethite specific surface area 7-12-2007.xls*
Carruthers et al. 1971 [DIRS 178656]	Figure 7	Water Vapor Adsorption Isotherms for chromium oxide gel	5 (a)	3, 10	Table 4.1-19, p. 4-33, Section 6.3.4.3.2, p. 6-72, Figure 6.3-34, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Corrosion Products Composite Isotherm 7-19-2007.xls*
	Table IV	Specific surface area for chromium oxide gel	5 (a)	3, 10	Table 4.1-19, p. 4-33, Section 6.3.4.3.3, Table 6.3-7

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Input	Source	Description	Method[1] (Rationale)[2]	Attribute[3]	Locations within AMR Where Data Are Listed and Where Qualification Is Documented or Corroboration Is Demonstrated
Morimoto et al. 1969 [DIRS 162877]	Figures 3 and 4 (adsorption isotherms) and Table I (monolayer capacity)	Water Vapor Adsorption Isotherms and monolayer capacity for α-Fe_2O_3	5 (a)	3, 10	Table 4.1-19, p. 4-33, Section 6.3.4.3.2, p. 6-72, Figure 6.3-34, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Corrosion Products Composite Isotherm 7-19-2007.xls*
Harju et al. 2005 [DIRS 178670]	Figure 4a (adsorption isotherm) and Table 6 (monolayer volume)	Water Vapor Adsorption Isotherm and monolayer volume for Cr_2O_3	5 (a)	3, 10	Table 4.1-19, p. 4-33, Section 6.3.4.3.2, p. 6-72, Figure 6.3-34, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Corrosion Products Composite Isotherm 7-19-2007.xls*
Rice et al. 1980 [DIRS 178725]	Figure 2	Water Vapor Adsorption Isotherms for NiO	5 (a)	3, 10	Table 4.1-19, p. 4-33, Section 6.3.4.3.2, p. 6-72, Figure 6.3-34, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Corrosion Products Composite Isotherm 7-19-2007.xls*
Nagao et al. 1995 [DIRS 162878]	Figure 1b	Water Vapor Adsorption Isotherm for Cr_2O_3	5 (a)	3, 10	Table 4.1-19, p. 4-33, Section 6.3.4.3.2, p. 6-72, Figure 6.3-34, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Corrosion Products Composite Isotherm 7-19-2007.xls*
	p. 222	Specific surface area for Cr_2O_3	5 (a)	3, 10	Table 4.1-19, p. 4-33, Section 6.3.4.3.3, Table 6.3-7
Kuwabara et al. 1987 [DIRS 178682]	Figure 1	Water Vapor Adsorption Isotherm for α-Fe_2O_3	5 (a)	3, 10	Table 4.1-19, p. 4-33, Section 6.3.4.3.2, p. 6-72, Figure 6.3-34, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Corrosion Products Composite Isotherm 7-19-2007.xls*
Kittaka et al. 1984 [DIRS 178830]	Figure 6a (adsorption isotherm) and p. 459 (monolayer covereage)	Water Vapor Adsorption Isotherm and monolayer coverage for α-$HCrO_2$	5 (a)	3, 10	Table 4.1-19, p. 4-33, Section 6.3.4.3.2, p. 6-72, Figure 6.3-34, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Corrosion Products Composite Isotherm 7-19-2007.xls*
	Table 1	Specific surface area for α-$HCrO_2$	5 (a)	3, 10	Table 4.1-19, p. 4-33, Section 6.3.4.3.3, Table 6.3-7

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Input	Source	Description	Method[1] (Rationale)[2]	Attribute[3]	Locations within AMR Where Data Are Listed and Where Qualification Is Documented or Corroboration Is Demonstrated
Kittaka et al. 1983 [DIRS 178681]	Figure 6, Figure 7 (adsorption isotherms) and Table 1 (monolayer capacity)	Water Vapor Adsorption Isotherms and monolayer capacity for Cr_2O_3	5 (a)	3, 10	Table 4.1-19, p. 4-33, Section 6.3.4.3.2, p. 6-72, Figure 6.3-34, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Corrosion Products Composite Isotherm 7-19-2007.xls*
	Table 1	Specific surface area for Cr_2O_3	5 (a)	3, 10	Table 4.1-19, p. 4-33, Section 6.3.4.3.3, Table 6.3-7
Micale et al. 1976 [DIRS 179136]	Figure 3 (adsorption isotherms) and p. 542 (statistical monolayer)	Water Vapor Adsorption Isotherms and statistical monolayer for $Ni(OH)_2$	5 (a)	3, 10	Table 4.1-19, p. 4-33, Section 6.3.4.3.2, p. 6-72, Figure 6.3-34, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Corrosion Products Composite Isotherm 7-19-2007.xls*
	p. 541 and 542	Specific surface area for $Ni(OH)_2$	5 (a)	3, 10	Table 4.1-19, p. 4-33, Section 6.3.4.3.3, Table 6.3-7
Micale et al. 1985 [DIRS 173785]	Figures 2 and 3 (adsorption isotherms) and Table 1 (monolayer coverage)	Water Vapor Adsorption Isotherm for α-Fe_2O_3 and γ-FeOOH	5 (a)	3, 10	Table 4.1-19, p. 4-33, Section 6.3.4.3.2, p. 6-72, Figure 6.3-34, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Corrosion Products Composite Isotherm 7-19-2007.xls*

Table 1. Data Qualification for External Source Data Qualified for Intended Use in Document ANL-WIS-PA-000001 REV 03 (Continued)

Input	Source	Description	Method[1] (Rationale)[2]	Attribute[3]	Locations within AMR Where Data Are Listed and Where Qualification Is Documented or Corroboration Is Demonstrated
Jurinak 1964 [DIRS 154381]	Figures 5 and 6	Water Vapor Adsorption Isotherms for α-Fe_2O_3 and FeOOH	5 (a)	3, 10	Table 4.1-19, p. 4-33, Section 6.3.4.3.2, p. 6-72, Figure 6.3-34, output DTN: SN0703PAEBSRTA.001 [DIRS 185343], file *Corrosion Products Composite Isotherm 7-19-2007.xls*
	Table 1	Specific surface area for α-Fe_2O_3 and FeOOH	5 (a)	3, 10	Table 4.1-19, p. 4-33, Section 6.3.4.3.3, Table 6.3-7

1 Method from SCI-PRO-001, *Qualification of Unqualified Data*, Attachment 2.
2 The rationale is that (a) it is the most suitable considering the data, the intended use, and availability of corroborating data; (b) it is the most suitable considering the use in similar applications; (c) it is the most suitable considering the data and available documentation of the QA program; (d) it is the most suitable considering the data and the existing documentation regarding the data and the data originator; (e) corroborating data are available for comparison with the unqualified data set and any inferences drawn to corroborate the unqualified data can be clearly identified, justified and documented.
3 Attributes from SCI-PRO-001, *Qualification of Unqualified Data*, Attachment 3.

Table 2. DIRS Changes to Correct Indirect/Direct Classification and Miscellaneous Related Changes

Input	Source	Description	DIRS Changes Required
McCafferty and Zettlemoyer 1970 [DIRS 154382]	Figure 3	Water vapor adsorption Isotherms for α-Fe_2O_3	In 3rd DIRS entry, change "Steel Corrosion Products" to "Fe2O3" under Input Description. Change input usage to "Direct Input" Change "N/A" to "Data" under Input Category.
	p. 453	Specific surface area of Fe_2O_3	In 2nd DIRS entry, delete "Entire," under Specifically Used From; delete "Sections 6.3.4.3.1, 6.3.4.3.2;" under Specifically Used In; delete ", adsorption isotherm for water vapor on Fe2O3" under Input Description.
	p. 454	Water molecule cross-sectional area, A_w	In 1st DIRS entry, change "6.3.4.3.3" to "6.3.4.3.2" under Specifically Used From;
Cornejo et al. 1984 [DIRS 178660]	Table 1	Specific surface area for HFO	Change input usage to "Direct Input" Change "N/A" to "Data" under Input Category.
Cornejo 1987 [DIRS 178659]	Table 1	Specific surface area for HFO	Change input usage to "Direct Input" Change "N/A" to "Data" under Input Category.
Schwertmann et al. 2004 [DIRS 178734]	Table 1	Specific surface area for HFO	Change input usage to "Direct Input" Change "N/A" to "Data" under Input Category.
Mitov et al. 2002 [DIRS 178686]	Table 5	Specific surface area for HFO	Change input usage to "Direct Input" Change "N/A" to "Data" under Input Category.
Clausen and Fabricius 2000 [DIRS 178655]	Table 2	Specific surface area for HFO	Change input usage to "Direct Input" Change "N/A" to "Data" under Input Category.
O'Reilly and Hochella 2003 [DIRS 178704]	Table 1	Specific surface area for HFO	Change input usage to "Direct Input" Change "N/A" to "Data" under Input Category.
Sani et al. 2004 [DIRS 178727]	p. 2640	Specific surface area for HFO	Change input usage to "Direct Input" Change "N/A" to "Data" under Input Category.
Hofmann et al. 2004 [DIRS 173783]	Table 1	Specific surface area for HFO	Change input usage to "Direct Input" Change "N/A" to "Data" under Input Category.
	Figure 8	Water Vapor Adsorption Isotherms for HFO	Delete 1st DIRS entry (Input Description: "Comparison of Adsorption Isotherms…"). In 3rd DIRS entry, add "Figure 6.3-23" under Specifically Used In; change "Steel Corrosion Products" to "HFO;" change input usage to "Direct Input" Change "N/A" to "Data" under Input Category.
	p. 167	Density of HFO	Change input usage to "Indirect Input." Change "Data" to "N/A" under Input Category.

Input | Source | Description | DIRS Changes Required

Table 2. DIRS Changes to Correct Indirect/Direct Classification and Miscellaneous Related Changes (Continued)

Input	Source	Description	DIRS Changes Required
Sauvé et al. 2000 [DIRS 178732]	Table 1	Specific surface area for HFO	Change input usage to “Direct Input” Change “N/A” to “Data” under Input Category.
Weidler 1997 [DIRS 178741]	Table 1	Specific surface area for HFO	Change input usage to “Direct Input” Change “N/A” to “Data” under Input Category.
Guzman et al. 1994 [DIRS 178669]	Table 1	Specific surface area for HFO	Change input usage to “Direct Input” Change “N/A” to “Data” under Input Category.
Larsen and Postma 2001 [DIRS 178683]	Table 2	Specific surface area for HFO	Change input usage to “Direct Input” Change “N/A” to “Data” under Input Category.
Leone et al. 2001 [DIRS 178684]	p. 1317	Specific surface area for HFO	Change input usage to “Direct Input” Change “N/A” to “Data” under Input Category.
Davis and Leckie 1978 [DIRS 125591]	p. 95	Specific surface area for HFO	Change input usage to “Direct Input” Change “N/A” to “Data” under Input Category.
Liaw et al. 1989 [DIRS 178685]	Table 1	Specific surface area for HFO	Change input usage to “Direct Input” Change “N/A” to “Data” under Input Category.
Crosby et al. 1983 [DIRS 178662]	Table II	Specific surface area for HFO	Change input usage to “Direct Input” Change “N/A” to “Data” under Input Category.
Axe and Anderson 1995 [DIRS 178654]	p. 159	Specific surface area for HFO	Change input usage to “Direct Input” Change “N/A” to “Data” under Input Category.
Van der Giessen 1966 [DIRS 178740]	Table 1	Specific surface area for HFO	Change input usage to “Direct Input” Change “N/A” to “Data” under Input Category.
Davies-Colley et al. 1984 [DIRS 178666]	p. 492	Specific surface area for HFO	Change input usage to “Direct Input” Change “N/A” to “Data” under Input Category.
Tipping 1981 [DIRS 178737]	Table 1	Specific surface area for HFO	Change input usage to “Direct Input” Change “N/A” to “Data” under Input Category.
Carlson and Schwertmann 1981 [DIRS 142788]	Table 1	Specific surface area for HFO	Change input usage to “Direct Input” Change “N/A” to “Data” under Input Category.
Eggleton and Fitzpatrick 1988 [DIRS 173878]	Table 1	Specific surface area for HFO	Change input usage to “Direct Input” Change “N/A” to “Data” under Input Category.
Turner and Sassman 1996 [DIRS 179618]	Tables 1 and 3	Surface Complexation Constants	Change input usage to “Direct Input” Change “N/A” to “Data” under Input Category.
Wang et al. 2001 [DIRS 176816]	Tables 3 and 4	Surface Complexation Constants	Change input usage to “Direct Input” Change “N/A” to “Data” under Input Category.

Input	Source	Description	DIRS Changes Required
Pepper et al.2006 [DIRS 179622]	Table 2	Surface Complexation Constants	Change input usage to "Direct Input" Change "N/A" to "Data" under Input Category.
Cromières et al. 1998 [DIRS 179616]	Table 4	Surface Complexation Constants	Change input usage to "Direct Input" Change "N/A" to "Data" under Input Category.
Appelo et al. 2002 [DIRS 168168]	Table 2	Surface Complexation Constants	Change input usage to "Direct Input" Change "N/A" to "Data" under Input Category.
LaVerne and Tandon 2003 [DIRS 178303]	Figure 1	Water Vapor Adsorption Isotherms for SNF Waste Form Materials	Change input usage to "Direct Input" Change "N/A" to "Data" under Input Category.
	p. 13624	Specific surface area for UO_2 and CeO_2	Change input usage to "Direct Input" Change "N/A" to "Data" under Input Category.
Gammage et al. 1970 [DIRS 178304]	Figure 2, p. 4277	Water Vapor Adsorption Isotherm and specific surface area for SNF waste form materials	Add "Specific surface area of ThO2" to Input Description. Change input usage to "Direct Input" Change "N/A" to "Data" under Input Category.
Holmes et al. 1974 [DIRS 154379]	Figure 3	Water Vapor Adsorption Isotherm for SNF waste form materials	In 1st DIRS entry, add "Sections 4.1.2, 6.3.4.3.2" under Specifically Used In. In 2nd DIRS entry, delete "p. 368" under Specifically Used From; delete "Sections 4.1.2, 6.3.4.3.2; Tables 6.3-7, 6.3-12" under Specifically Used In; delete "Cross sectional area of a water molecule. Specific surface area of ZrO2." under Input Description; and change input usage to "Direct Input." Change "N/A" to "Data" under Input Category.
	p. 368 (specific surface area)	Specific surface area of ZrO_2.	In 3rd DIRS entry, delete "Fig. 3 (adsorption isotherm)" under Specifically Used From; add "Tables 6.3-7, 6.3-12" under Specifically Used In; delete "Water Vapor Adsorption Isotherms for SNF Waste Form Materials" and add "Specific surface area of ZrO2" under Input Description; and change input usage to "Direct Input." Change "N/A" to "Data" under Input Category.
Stakebake 1971 [DIRS 178302]	Figure 8	Water Vapor Adsorption Isotherm for SNF waste form materials	In 1st DIRS entry, delete ",p. 253 (specific surface area)" under Specifically Used From; add "Figure 6.3-38" under Specifically Used In; add "(PuO2)" under Input Description; change input usage to "Direct Input" Change "N/A" to "Data" under Input Category.

Input	Source	Description	DIRS Changes Required
	p. 253	Specific surface area of PuO_2.	In 2nd DIRS entry, add “(specific surface area)” under Specifically Used From; add “Table 4.1-18” under Specifically Used In; add “(specific surface area of PuO_2).” under Input Description; change input usage to “Direct Input” Change “N/A” to “Data” under Input Category. Delete 3rd DIRS entry (entire row).
Stakebake and Dringman 1968 [DIRS 178840]	Figure 3, Figure 4, Table 1	Water Vapor Adsorption Isotherm and specific surface area for SNF waste form materials	Change input usage to “Direct Input” Change “N/A” to “Data” under Input Category.
Paffett et al. 2003 [DIRS 178712]	Figure 8, Table 1	Water Vapor Adsorption Isotherm and specific surface area for SNF waste form materials	Change input usage to “Direct Input” Change “N/A” to “Data” under Input Category.
Kandori and Ishikawa 1991 [DIRS 178680]	Figure 2	Water Vapor Adsorption Isotherm for amorphous ferric oxide hydroxide	Change input usage to “Direct Input” Change “N/A” to “Data” under Input Category.
Koch and Møller 1987 [DIRS 173784]	Figures 5 and 6	Water Vapor Adsorption Isotherms for goethite	In 2nd DIRS entry, delete “; Table 1 (specific surface area)” under Specifically Used From; add “Figures 6.3-21, 6.3-22” under Specifically Used In; add “ (Goethite)” under Input Description; Change input usage to “Direct Input” Change “N/A” to “Data” under Input Category.
	Table 1	Goethite specific surface area	In 3rd DIRS entry, delete “Figures 5 and 6” and add ”Table 1 (specific surface area)” under Specifically Used From; delete “Figures 6.3-21, 6.3-22” and add “Table 4.1-19” under Specifically Used In; delete “Water Vapor Adsorption Isotherm for Goethite” and add “Specific surface area of goethite” under Input Description; change input usage to “Direct Input” Change “N/A” to “Data” under Input Category.
Carruthers et al. 1971 [DIRS 178656]	Figure 7	Water Vapor Adsorption Isotherms for chromium oxide gel	In 1st DIRS entry, change input usage to “Direct Input” Change “N/A” to “Data” under Input Category.
	Table IV	Specific surface area for chromium oxide gel	In 1st DIRS entry, add “Specific surface area of chromium oxide gel.” under Input Description;

Input	Source	Description	DIRS Changes Required
Morimoto et al. 1969 [DIRS 162877]	Figures 3 and 4 (adsorption isotherms) and Table I (monolayer capacity)	Water Vapor Adsorption Isotherms and monolayer capacity for α-Fe_2O_3	Change input usage to “Direct Input” Change “N/A” to “Data” under Input Category.
Harju et al. 2005 [DIRS 178670]	Figure 4a (adsorption isotherm) and Table 6 (monolayer volume)	Water Vapor Adsorption Isotherm and monolayer volume for Cr_2O_3	Change input usage to “Direct Input” Change “N/A” to “Data” under Input Category.
Rice et al. 1980 [DIRS 178725]	Figure 2	Water Vapor Adsorption Isotherms for NiO	Change input usage to “Direct Input” Change “N/A” to “Data” under Input Category.
Nagao et al. 1995 [DIRS 162878]	Figure 1b, p. 222	Water Vapor Adsorption Isotherm and specific surface area for Cr_2O_3	Change input usage to “Direct Input” Change “N/A” to “Data” under Input Category.
Kuwabara et al. 1987 [DIRS 178682]	Figure 1	Water Vapor Adsorption Isotherm for α-Fe_2O_3	Change input usage to “Direct Input” Change “N/A” to “Data” under Input Category.
Kittaka et al. 1984 [DIRS 178830]	Figure 6a (adsorption isotherm) and p. 459 (monolayer covereage)	Water Vapor Adsorption Isotherm and monolayer coverage for α-$HCrO_2$	Change input usage to “Direct Input” Change “N/A” to “Data” under Input Category.
	Table 1	Specific surface area for α-$HCrO_2$	Change input usage to “Direct Input” Change “N/A” to “Data” under Input Category.
Kittaka et al. 1983 [DIRS 178681]	Figure 6, Figure 7 (adsorption isotherms) and Table 1 (monolayer capacity)	Water Vapor Adsorption Isotherms and monolayer capacity for Cr_2O_3	Change input usage to “Direct Input” Change “N/A” to “Data” under Input Category.
	Table 1	Specific surface area for Cr_2O_3	Change input usage to “Direct Input” Change “N/A” to “Data” under Input Category.
Micale et al. 1976 [DIRS 179136]	Figure 3 (adsorption isotherms) and p. 542 (statistical monolayer)	Water Vapor Adsorption Isotherms and statistical monolayer for $Ni(OH)_2$	Change input usage to “Direct Input” Change “N/A” to “Data” under Input Category.
	p. 541 and 542	Specific surface area for $Ni(OH)_2$	Change input usage to “Direct Input” Change “N/A” to “Data” under Input Category.
Micale et al. 1985 [DIRS 173785]	Figures 2 and 3 (adsorption isotherms) and Table 1 (monolayer coverage)	Water Vapor Adsorption Isotherm for α-Fe_2O_3 and γ-FeOOH	Change input usage to “Direct Input” Change “N/A” to “Data” under Input Category.
Bear 1988 [DIRS 101379]	p. 116	Exponents used in Archie’s law	Change input category to “Established Fact”
Langmuir 1997 [DIRS 100051]	Table 10.2	Specific surface area of hematite	Change input category to “Established Fact”
Cornell and Schwertmann 2003 [DIRS 173037]	Entire	Density of HFO	Change input usage to “Indirect Input” Change “Data” to “N/A” under Input Category.

Input	Source	Description	DIRS Changes Required
Christl and Kretzschmar 1999 [DIRS 173811]	p. 2929	Site densities can be measured or estimated through fitting in a SCM.	Change input usage to "Indirect Input" Change "Data" to "N/A" under Input Category.
Hofmann et al. 2005 [DIRS 173711]	Table 2	Surface area and site density for HFO.	Change input usage to "Indirect Input" Change "Data" to "N/A" under Input Category.
Reimus et al. 2002 [DIRS 163008]	p. 2.25, Equation 2.5	Diffusion coefficient for saturated whole rock samples of tuff.	Delete "Table 4.1-19," and change "Sections 4.1.2, 6.5.3.6, 6.6.4.2" to "Section 6.6.4.2." Change input usage to "Indirect Input" Change "Data" to "N/A" under Input Category.
Jurinak 1964 [DIRS 154381]	Figures 5 and 6	Water Vapor Adsorption Isotherms for α-Fe_2O_3 and FeOOH	In 1st DIRS entry, replace "p. 480" with "pp. 479-480" under Specifically Used From; delete "Figures 6.3-7 & 7.2-1" under Specifically Used In; replace "Water adsorption isotherm on Fe2O3" with "Water molecule cross sectional area" under Input Description; change input usage to "Indirect Input." Change "Data" to "N/A" under Input Category. In 2nd DIRS entry, change "Figure 6" to "Figures 5 and 6" under Specifically Used From; change "Figure 6.3-20" to "Figures 6.3-19 and 6.3-20" under Specifically Used In; delete "Water molecule cross sectional area; specific surface area of Fe2O3" and "goethite specific surface area" and replace "Goethite water adsorption isotherm" with "Goethite and Fe2O3 water adsorption isotherms" under Input Description; change input usage to "Direct Input" Change "N/A" to "Data" under Input Category.
	Table I	Specific surface area for α-Fe_2O_3 and FeOOH	In 3rd DIRS entry, change "Fig. 5" to "Table I" under Specifically Used From; delete "; Figure 6.3-19" under Specifically Used In; change "Water Vapor Adsorption Isotherms for Steel Corrosion Products" to "Specific surface area of Fe2O3 and goethite" under Input Description; change input usage to "Direct Input" Change "N/A" to "Data" under Input Category. Delete 4th DIRS entry (Input Description "'Close-packed' monolayer of water").

Input	Source	Description	DIRS Changes Required
Dzombak and Morel 1990 [DIRS 105483]	Table 5.3	Sorption density and specific surface area data for ferrihydrite	Change input category to “Established Fact”
	Table 10.5	Surface Complexation Constants	Change input usage to “Direct Input” and input category to “Established Fact”
Briand et al. 2001 [DIRS 161617]	Table 4	Specific surface area of Fe_2O_3	Change input category to “Indirect Input” Change “Data” to “N/A” under Input Category.
Mills 1973 [DIRS 133392]	Table III	Self-diffusion coefficient of water	Change input category to “Indirect input” Change “Data” to “N/A” under Input Category.

V. CR 13657 Resolution

CR 13657 is resolved by correcting references in Figures 7.2-13 and 7.2-14 and providing specific locations of data in the sources:

1. In Figure 7.2-13, change the reference in the "Sources" notation from "EPA 2004 [DIRS 170376]" to "EPA 2004 [DIRS 172215], Table 5.22" and change the reference in the figure title from "EPA 1999 [DIRS 170376]" to "EPA 2004 [DIRS 172215], Table 5.22."

2. In Figure 7.2-14, change the reference in the "Sources" notation from "EPA 2004 [DIRS 170376]" to "EPA 2004 [DIRS 172215], Table 5.6."

None of the changes in response to CR 13657 impacts the conclusions of ANL-WIS-PA-000001 REV 03, and no downstream usage—neither the LA nor other project documents—is impacted.

VI. CR 13740 Resolution

CR 13740 is resolved by changing the word "highest" to "lowest" in describing the concentration of competing cations in the validation of the competitive surface complexation model in ANL-WIS-PA-000001 REV 03, Section 7.2.3:

1. p. 7-37, last 2 lines, and p. 7-38, 1st line: Change "The higher K_ds from the C-SCM are typically calculated when multiple extrema of the model are sampled (e.g., the highest surface areas, the lowest values, the highest concentration of competing cations)" to "The higher K_ds from the C-SCM are typically calculated when multiple extrema of the model are sampled (e.g., the highest surface areas, the lowest P_{CO_2} values, the lowest concentration of competing cations)."

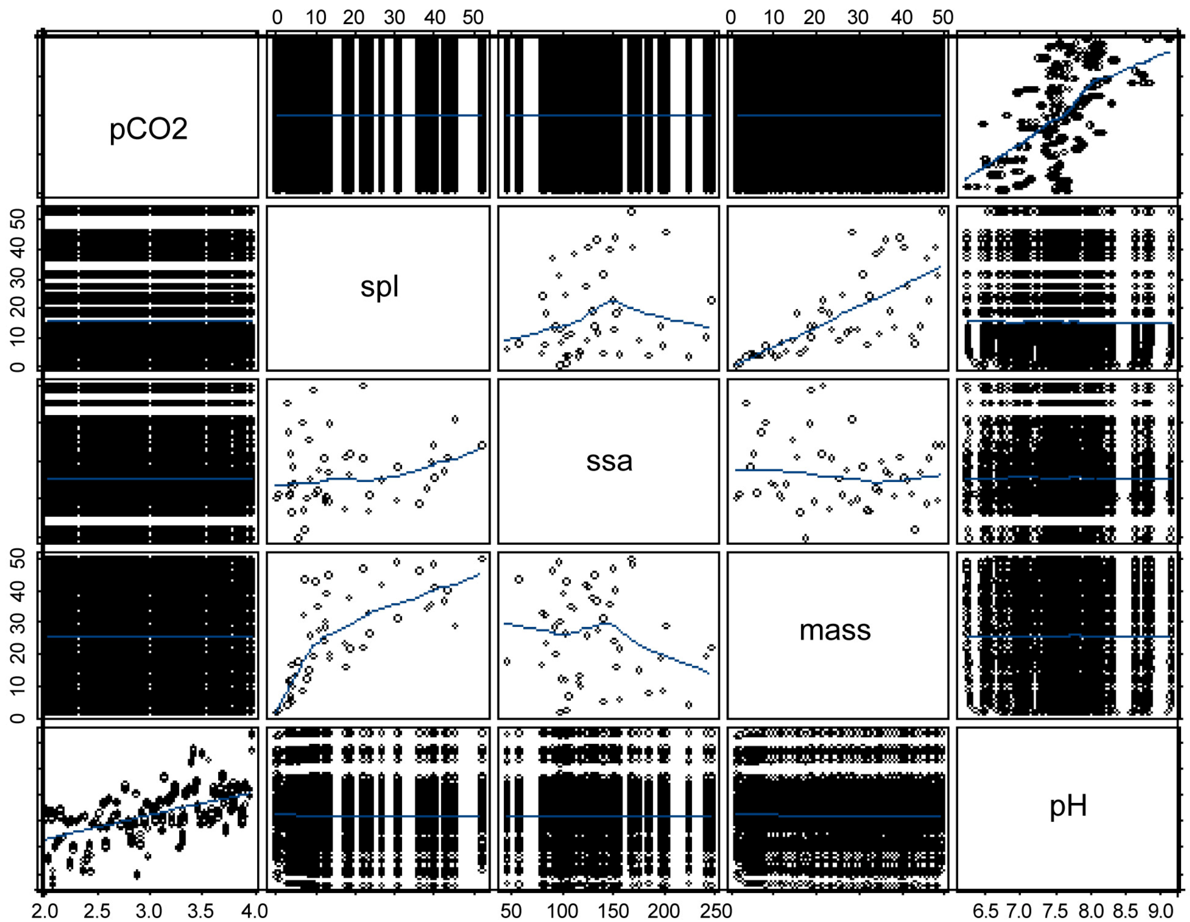
2. p. 7-40, 1st paragraph under **Neptunium** heading, next-to-last sentence: Change "The higher K_ds from the C-SCM are calculated when multiple extrema of the model are sampled (e.g., the highest surface areas, the lowest P_{CO_2} values, the highest concentration of competing cations)" to "The higher K_ds from the C-SCM are calculated when multiple extrema of the model are sampled (e.g., the highest surface areas, the lowest P_{CO_2} values, the lowest concentration of competing cations)."

3. p. 7-41, lines 6-8: Change "The higher Am K_ds are calculated when multiple extrema of the model are sampled (e.g., the highest surface areas, the lowest P_{CO_2} values, the highest concentration of competing cations)" to "The higher Am K_ds are calculated when multiple extrema of the model are sampled (e.g., the highest surface areas, the lowest P_{CO_2} values, the lowest concentration of competing cations)."

These statements are only utilized as discussion of the information and are not used to constrain the values utilized within the safety analysis. None of the changes in response to CR 13740 impacts the conclusions of ANL-WIS-PA-000001 REV 03 and no downstream usage—neither the LA nor other project documents—is impacted.

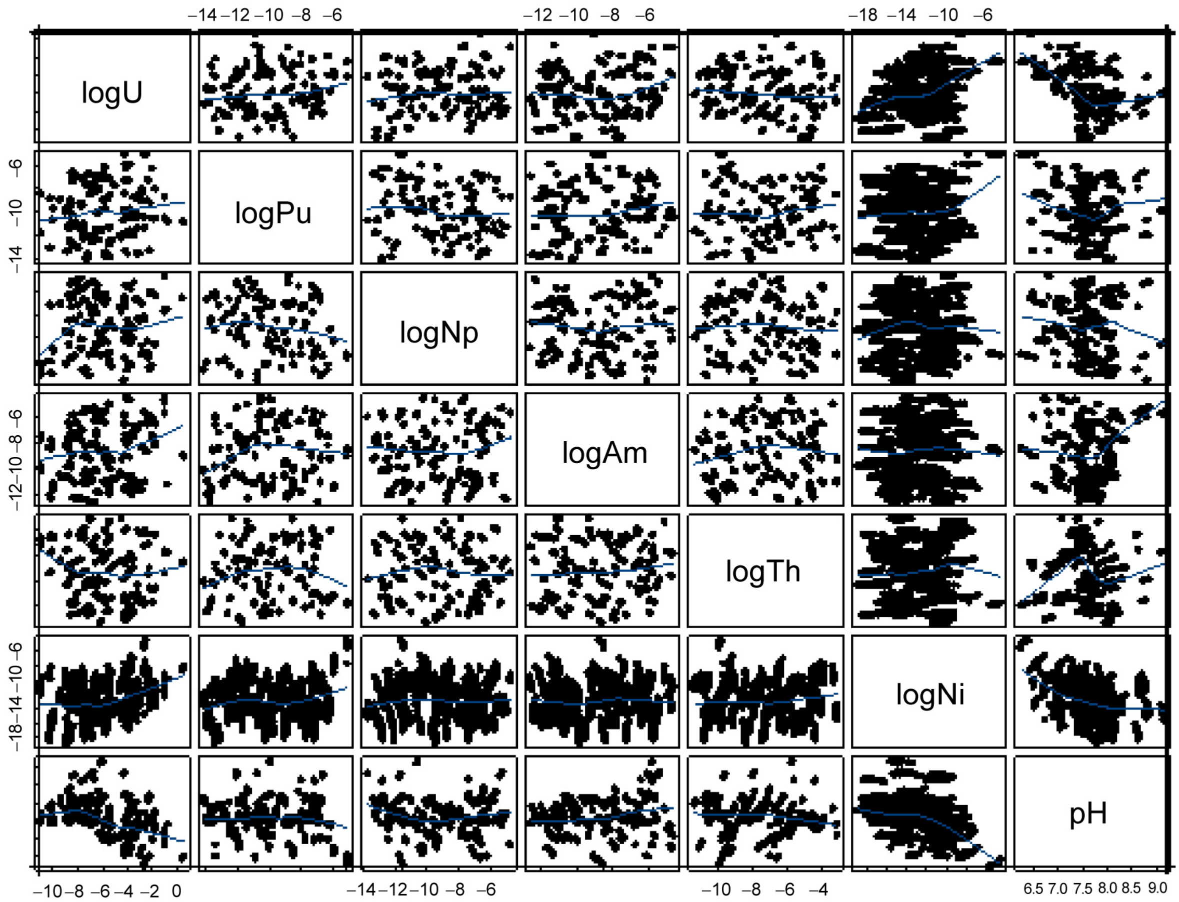
VII. CR 13678 Resolution

CR 13678 is resolved by replacing Figures 6.5-10 and 6.5-11, in which image resolution is poor and figure and axis labels are illegible, with the following figures having better resolution and legible figure and axis labels. (Note that the thick bands in Figure 6.5-10 are the result of the density and orientation of data points and are not an indication of low resolution in the plots.)



Source: S-PLUS plot of data in output DTN: SN0703PAEBSRTA.002

Figure 6.5-10. Scatter Plot Matrix of First 5 Predictors Versus the pH Response



Source: S-PLUS plot of data in output DTN: SN0703PAEBSRTA.002

Figure 6.5-11. Scatter Plot Matrix of 6 Dissolved Concentration Predictors Versus the pH Response

None of the changes in response to CR 13678 impacts the conclusions of ANL-WIS-PA-000001 REV 03 and no downstream usage—neither the LA nor other project documents—is impacted.

VIII. CR 13643 Resolution

CR 13643 is resolved by correcting Eq. 6.5.1.2-9, which makes it consistent with the correct implementation in the TSPA-LA. In addition, the text describing Eq. 6.5.1.2-9 is corrected and revised to provide a clearer explanation of the concentration term. This correction also affects Eqs. 6.5.1.2-39 and 6.5.1.2-47 in Section 6.5.1.2 along with text and Eqs. 6.5.2.5-10 to 6.5.2.5-12 in Section 6.5.2.5.

None of the changes in response to CR 13643 impacts the conclusions of ANL-WIS-PA-000001 REV 03 and no downstream usage—neither the LA nor other project documents—is impacted.

CR 13643 is resolved by the following changes (in which underlining indicates the original text to be changed and the revised text):

1. p. 6-149, Eq. 6.5.1.2-9 and associated text: Change:

The term Q_{icm}^{embed} is the rate of mass conversion from dissolved state to embedded state onto waste form colloids for radionuclide species *i*. Radionuclides become embedded only in waste form colloids, not in iron oxyhydroxide or groundwater colloids. The conversion rate to embedded species is represented by a first order conversion of the species in solution:

$$Q_{icm}^{embed} = \theta_w \lambda_i^{embed} C_i , \qquad \text{(Eq. 6.5.1.2-9)}$$

where λ_i^{embed} is the first order rate constant (s^{-1}) for mass conversion from the dissolved state to the embedded state onto waste form colloids for radionuclide species *i*.

to:

For the waste form colloids generated during the degradation of the HLW glass and CSNF matrix, some mass of plutonium and americium is considered to be "embedded" within the waste form colloids at the time of generation and thereby considered as an intrinsic part of the colloid, not in equilibrium with the aqueous system. The term Q_{icm}^{embed} is the rate of conversion of mass of species *i* from degradation of the waste form to the embedded state associated the waste form colloids. The conversion rate to the embedded state is represented by a first order conversion:

$$Q_{icm}^{embed} = \theta_w \lambda_i^{embed} C_i^* , \qquad \text{(Eq. 6.5.1.2-9)}$$

where λ_i^{embed} is the first order rate constant (s^{-1}) for conversion of degraded mass of species *i* to the embedded mass associated with waste form colloids and the concentration term, C_i^*, is the concentration based on the mass of radionuclide species *i* made available from the degradation of the waste form per unit volume of water. This equation is discussed further in Section 6.5.2.5, where discretization of the mass balance equations and implementation in the TSPA are described. Radionuclides are considered to be embedded only in waste form colloids, not in iron oxyhydroxide or groundwater colloids.

2. p. 6-157, Eq. 6.5.1.2-39: Change:

$$\begin{aligned}\frac{\partial}{\partial t}\left[\theta_w R_{fi} C_i\right] &= \nabla \cdot \left(\theta_w D_i \nabla C_i\right) \\ &+ \nabla \cdot \left\{\theta_w D_c \nabla\left[\left(K_{dicWF} C_{cWF} + K_{dicFeO} C_{cFeO} + K_{dicGW} C_{cGW}\right) C_i\right]\right\} \\ &- \nabla \cdot \left[\boldsymbol{q}_w \left(1 + K_{dicWF} C_{cWF} + K_{dicFeO} C_{cFeO} + K_{dicGW} C_{cGW}\right) C_i\right] \qquad \text{(Eq. 6.5.1.2-39)} \\ &\pm Q_{idp} - \left(\rho_b \bar{s}_{CP} + \theta_w C_{cFeO} \bar{s}_{cFeO}\right) k_{if} C_i + \rho_b \bar{s}_{CP} k_{ir} \hat{C}_{iCP} - \theta_w \lambda_i^{embed} C_i \\ &+ \theta_w \left[\lambda_i^p r_{Mi}^p R_{fi}^p C_i^p - \lambda_i R_{fi} C_i\right],\end{aligned}$$

to:

$$\frac{\partial}{\partial t}\left[\theta_w R_{fi} C_i\right] = \nabla \cdot \left(\theta_w D_i \nabla C_i\right)$$
$$+ \nabla \cdot \left\{\theta_w D_c \nabla\left[\left(K_{dicWF} C_{cWF} + K_{dicFeO} C_{cFeO} + K_{dicGW} C_{cGW}\right) C_i\right]\right\}$$
$$- \nabla \cdot \left[\boldsymbol{q}_w \left(1 + K_{dicWF} C_{cWF} + K_{dicFeO} C_{cFeO} + K_{dicGW} C_{cGW}\right) C_i\right] \qquad \text{(Eq. 6.5.1.2-39)}$$
$$\pm Q_{idp} - \left(\rho_b \bar{s}_{CP} + \theta_w C_{cFeO} \bar{s}_{cFeO}\right) k_{if} C_i + \rho_b \bar{s}_{CP} k_{ir} \hat{C}_{iCP} - \theta_w \lambda_i^{embed} C_i^*$$
$$+ \theta_w \left[\lambda_i^p r_{Mi}^p R_{fi}^p C_i^p - \lambda_i R_{fi} C_i\right],$$

[Note: The only change is in the last term in the 4th line, where C_i is replaced with C_i^*.]

3. p. 6-159, Eq. 6.5.1.2-47: Change:

$$\frac{\partial}{\partial t}\left[\theta_w R_{fi} C_i\right] = \frac{\partial}{\partial z}\left(\theta_w D_i \frac{\partial C_i}{\partial z}\right)$$
$$+ \frac{\partial}{\partial z}\left(\theta_w D_c \frac{\partial}{\partial z}\left[\left(K_{dicWF} C_{cWF} + K_{dicFeO} C_{cFeO} + K_{dicGW} C_{cGW}\right) C_i\right]\right)$$
$$- \frac{\partial}{\partial z}\left[q_{wz}\left(1 + K_{dicWF} C_{cWF} + K_{dicFeO} C_{cFeO} + K_{dicGW} C_{cGW}\right) C_i\right] \qquad \text{(Eq. 6.5.1.2-47)}$$
$$\pm Q_{idp} - \left(\rho_b \bar{s}_{CP} + \theta_w C_{cFeO} \bar{s}_c\right) k_{if} C_i + \rho_b \bar{s}_{CP} k_{ir} \hat{C}_{iCP} - \lambda_i^{embed} C_i$$
$$+ \theta_w \left[\lambda_i^p r_{Mi}^p R_{fi}^p C_i^p - \lambda_i R_{fi} C_i\right].$$

to:

$$\frac{\partial}{\partial t}\left[\theta_w R_{fi} C_i\right] = \frac{\partial}{\partial z}\left(\theta_w D_i \frac{\partial C_i}{\partial z}\right)$$
$$+ \frac{\partial}{\partial z}\left(\theta_w D_c \frac{\partial}{\partial z}\left[\left(K_{dicWF} C_{cWF} + K_{dicFeO} C_{cFeO} + K_{dicGW} C_{cGW}\right) C_i\right]\right)$$
$$- \frac{\partial}{\partial z}\left[q_{wz}\left(1 + K_{dicWF} C_{cWF} + K_{dicFeO} C_{cFeO} + K_{dicGW} C_{cGW}\right) C_i\right] \qquad \text{(Eq. 6.5.1.2-47)}$$
$$\pm Q_{idp} - \left(\rho_b \bar{s}_{CP} + \theta_w C_{cFeO} \bar{s}_c\right) k_{if} C_i + \rho_b \bar{s}_{CP} k_{ir} \hat{C}_{iCP} - \lambda_i^{embed} C_i^*$$
$$+ \theta_w \left[\lambda_i^p r_{Mi}^p R_{fi}^p C_i^p - \lambda_i R_{fi} C_i\right].$$

[Note: The only change is in the last term in the 4th line, where C_i is replaced with C_i^*.]

4. p. 6-220, 2nd paragraph from bottom: Change:

Within the waste form domain, some part of the dissolved mass of plutonium and americium made available from the degradation of HLW glass and CSNF is converted to "embedded" mass on the waste form colloids. This conversion is required to satisfy the condition that some mass of plutonium and americium is "embedded" as an intrinsic part of the colloid and is not in equilibrium with the aqueous system, when generated from the degradation of HLW glass and

CSNF. This mass is thus transported separately as a distinct species [*Waste Form and In-Drift Colloids-Associated Radionuclide Concentrations: Abstraction and Summary* (BSC 2005 [DIRS 177423], Sections 6.3.1 & 6.3.3.3)]. The mass rate of conversion per unit volume of water is modeled as a first order reaction given by $\lambda_i^{embed} C_i$, where λ_i^{embed} is the linear rate constant, and concentration C_i is the dissolved concentration of plutonium and americium species in the waste form domain. The conversion rate λ_i^{embed} is calculated at each time step in the waste form domain. Its calculation is discussed below.

to:

Within the waste form domain, some part of the mass of plutonium and americium made available from the degradation of HLW glass and CSNF is converted to "embedded" mass associated with the waste form colloids. This "embedded" mass is considered to be an intrinsic part of the colloids and is assumed to be available to the waste form colloids as long as there is plutonium and americium present in the waste form domain. This mass is thus transported separately as a distinct species [*Waste Form and In-Drift Colloids-Associated Radionuclide Concentrations: Abstraction and Summary* (BSC 2005 [DIRS 177423], Sections 6.3.1 & 6.3.3.3)]. The mass rate of conversion per unit volume of water is modeled as a first order reaction given by $\lambda_i^{embed} C_i^*$ (Eq. 6.5.1.2-9), where λ_i^{embed} is the linear rate constant, and the concentration C_i^* is the mass of radionuclide species *i* in the waste form domain per unit volume of water. The conversion rate λ_i^{embed} is calculated at each time step in the waste form domain. Its calculation is discussed below.

5. p. 6-221, Eqs. 6.5.2.5-10 to 6.5.2.5-12: Change:

$$\frac{\partial\left(\theta_w C_i^{embed}\right)}{\partial t} = -Q_{adv/diff}^{wfc} \frac{C_i^{embed}}{C_{cWF}} + \lambda_i^{embed} \theta_w C_i . \qquad \text{(Eq. 6.5.2.5-10)}$$

Discretization of this equation gives:

$$\frac{(\theta_w C_i^{embed})^{n+1} - (\theta_w C_i^{embed})^n}{t^{n+1} - t^n} = -\left(Q_{adv/diff}^{wfc} \frac{C_i^{embed}}{C_{cWF}}\right)^n + \lambda_i^{embed} (\theta_w C_i)^n . \text{(Eq. 6.5.2.5-11)}$$

This equation is solved for the conversion rate:

$$\lambda_i^{embed} = \frac{\dfrac{\left(\theta_w C_i^{embed}\right)^{n+1} - \left(\theta_w C_i^{embed}\right)^n}{\Delta t} + \left(Q_{adv/diff}^{wfc} \dfrac{C_i^{embed}}{C_{cWF}}\right)^n}{\left(\theta_w C_i\right)^n} . \qquad \text{(Eq. 6.5.2.5-12)}$$

to:

$$\frac{\partial\left(\theta_w C_i^{embed}\right)}{\partial t} = -Q_{adv/diff}^{wfc} \frac{C_i^{embed}}{C_{cWF}} + \lambda_i^{embed} \theta_w C_i^* . \qquad \text{(Eq. 6.5.2.5-10)}$$

Discretization of this equation gives:

$$\frac{(\theta_w C_i^{embed})^{n+1} - (\theta_w C_i^{embed})^n}{t^{n+1} - t^n} = -\left(Q_{adv/diff}^{wfc} \frac{C_i^{embed}}{C_{cWF}}\right)^n + \lambda_i^{embed} (\theta_w C_i^*)^n . \qquad \text{(Eq. 6.5.2.5-11)}$$

This equation is solved for the conversion rate:

$$\lambda_i^{embed} = \frac{\dfrac{\left(\theta_w C_i^{embed}\right)^{n+1} - \left(\theta_w C_i^{embed}\right)^n}{\Delta t} + \left(Q_{adv/diff}^{wfc} \dfrac{C_i^{embed}}{C_{cWF}}\right)^n}{\left(\theta_w C_i^*\right)^n} . \qquad \text{(Eq. 6.5.2.5-12)}$$

[Note: The only changes are in the terms $\theta_w C_i$ (last term on the right in Eqs. 6.5.2.5-10 and 6.5.2.5-11 and in the denominator in Eq. 6.5.2.5-12), where C_i is replaced with C_i^*.]

6. Appendix A Notation, p. A-2, following definition of C_i: Add:

C_i^*	Concentration of radionuclide species *i* based on total mass of radionuclide species *i* in all states present in the waste form	kg m^{-3}	Eq. 6.5.1.2-9

IX. References

This section lists references that are used to resolve CRs in this ERD. References that are associated with a CR issue but are not used to resolve a CR, such as those in Tables 1 and 2, are not listed in this section.

IX.1. Documents Cited

169988 BSC (Bechtel SAIC Company) 2004. *Defense HLW Glass Degradation Model.* ANL-EBS-MD-000016 REV 02. Las Vegas, Nevada: Bechtel SAIC Company. ACC: DOC.20041020.0015; DOC.20050922.0002; LLR.20080408.0271; DOC.20081021.0002; DOC.20090323.0002.

111028 Ebert, W.L.; Hoburg, R.F.; and Bates, J.K. 1991. "The Sorption of Water on Obsidian and a Nuclear Waste Glass." *Physics and Chemistry of Glasses, 32,* (4), 133-137. Sheffield, England: Society of Glass Technology. TIC: 246078.

111034 Hagymassy, J., Jr.; Brunauer, S.; and Mikhail, R.Sh. 1969. "Pore Structure Analysis by Water Vapour Absorption. Part 1. T-Curves for Water Vapour." *Journal of Colloid and Interface Science, 29,* (3), 485-491. New York, New York: Academic Press. TIC: 246076.

177407 SNL (Sandia National Laboratories) 2007. *EBS Radionuclide Transport Abstraction.* ANL-WIS-PA-000001 REV 03. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20071004.0001; LLR.20080414.0023.

183478 SNL 2008. *Total System Performance Assessment Model /Analysis for the License Application.* MDL-WIS-PA-000005 REV 00 AD 01. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20080312.0001; LLR.20080414.0037; LLR.20080507.0002; LLR.20080522.0113; DOC.20080724.0005.

IX.2. Software Codes

182102 EXDOC_LA V. 2.0. 2007. WINDOWS XP, WINDOWS 2000 & WINDOWS 2003. STN: 11193-2.0-00.

184387 GoldSim V. 9.60.300. 2008. WIN 2000, WINXP, WIN2003. STN: 10344-9.60-03.

181049 MView V. 4.0. 2007. WINDOWS XP. STN: 10072-4.0-01.

185868 PHREEQC V. 2.11.01. 2008. WIN 2000. STN: 10068-2.11-01.

IX.3. Source Data, Listed by Data Tracking Number

185343 SN0703PAEBSRTA.001. Inputs Used in the Engineered Barrier System (EBS) Radionuclide Transport Abstraction. Submittal date: 04/10/2008.

IX.4. Output Data

MO0812TSPAOSIA.000. Over Sorption Impact Assessment for ERD-02 to ANL-WIS-PA-000001, Rev 03. Submittal date: 12/08/2008.

Attachment I – New DIRS Entries

Input Document			4. Specifically Used In:	5. Input Description	6. Input Usage	7. Input Category	8. Q Status	9. TBV/TBD Status
2a.	2. Technical Product Input Source Title and Identifier(s) with Version	3. Specifically Used From:						
352	SNL (Sandia National Laboratories) 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. 179466	Table 4-1; Parameter 01-10	Appendix I.1	Drift diameter	Indirect Input	N/A	N/A	N/A
353	SNL (Sandia National Laboratories) 2007. *Total System Performance Assessment Data Input Package for Requirements Analysis for Transportation Aging and Disposal Canister and Related Waste Package Physical Attributes Basis for Performance Assessment.* TDR-TDIP-ES-000006 REV 00. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20070918.0005; LLR.20080328.0012. 179394	Tables A-1 and A-3	Section 6.3.4.3.4.2; Table 6.3-10	Typical measurements and surface areas for 21-PWR TAD waste package components	Indirect Input	N/A	N/A	N/A
	SNL (Sandia National Laboratories) 2008. *Total System Performance Assessment Model /Analysis for the License Application.* MDL-WIS-PA-000005 REV 00 AD 01. Las Vegas, Nevada: Sandia National Laboratories. ACC: DOC.20080312.0001; LLR.20080414.0037; LLR.20080507.0002; LLR.20080522.0113; DOC.20080724.0005. 183478	Section 4[a]	ERD 02, Section II.1	Inputs to the models run for the analysis of over-prediction of sorption	Direct Input	Data	N/A	N/A
		Section 3[a]	ERD 02, Section II.2	Software used for the analysis of over-prediction of sorption is same as used in TSPA-LA	Indirect Input	N/A	N/A	N/A
	EXDOC_LA V. 2.0. 2007. WINDOWS XP, WINDOWS 2000 & WINDOWS 2003. STN: 11193-2.0-00. 182102	Entire	ERD 02, Section II.2	Used to calculate expected values for quantities of interest.	Direct Input	Qualified Software	N/A	N/A
	GoldSim V. 9.60.300. 2008. WIN 2000, WINXP, WIN2003. STN: 10344-9.60-03. 184387	Entire	ERD 02, Section II.2	Used to query TSPA baseline simulations and to perform sensitivity analyses with the TSPA model.	Direct Input	Qualified Software	N/A	N/A
	MView V. 4.0. 2007. WINDOWS XP. STN: 10072-4.0-01. 181049	Entire	ERD 02, Section II.2	Used for performing regression analyses based on TSPA results.	Direct Input	Qualified Software	N/A	N/A
	PHREEQC V. 2.11.01. 2008. WIN 2000. STN: 10068-2.11-01. 185868	Entire	ERD 02, Section II.2	Used to perform geochemical modeling and to evaluate the effects of major ions that compete for sorption sites.	Direct Input	Qualified Software	N/A	N/A
	Hagymassy, J., Jr.; Brunauer, S.; and Mikhail, R.Sh. 1969. "Pore Structure Analysis by Water Vapour Absorption. Part 1. T-Curves for Water Vapour." *Journal of Colloid and Interface Science*, *29*, (3), 485-491. New York, New York: Academic Press. TIC: 246076 111034	p. 489	ERD 02, Section IV	Isotherm for water on silica and quartz.	Indirect Input	N/A	N/A	N/A

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