# Model
# Error Resolution Document

*Complete only applicable items.*

QA: QA


**INITIATION**

| 1. Originator: Wendy A. Mitcheltree/David C. Sassani | 2. Date: 05/06/2008 | 3. ERD No. ANL-EBS-MD-000045 ERD 02 |
|---|---|---|
| 4. Document Identifier: ANL-EBS-MD-000045 Rev 03 | 5. Document Title: In-Drift Precipitates/Salts Model | |

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

Description:

This Error Resolution Document (ERD) is generated to address CR 11102. This ERD evaluates the issues listed in CR 11102 and provides corrections to errors that have been identified therein, or identified in the document during the corrective actions being performed.

As indicated in the pages below, CR 11102 contained multiple issues related to audit recommendations on the In-Drift Precipitates/Salts Model, ANL-EBS-MD-000045 Rev 03. These issues are evaluated below individually in the body of this ERD. In the cases where downstream reports had to be examined and evaluated for potential impacts from changes being made within this ERD, those documents are also listed within the "Evaluation" section for that particular issue.

There has been a clarifying note added to the file "readme.doc" from DTN: SN0609T0502404.012.

Justification:

In the attached materials it has been determined that none of the corrections affect the conclusions of the original product and have no impact to the downstream work that has been performed. There is no impact to the conclusion of this AMR and this ERD sufficiently corrects the issues for CR 11102 as detailed below:

**CONCURRENCE**

| | Printed Name | Signature | Date |
|---|---|---|---|
| 7. Checker | Susan E. Boggs | S Boggs | 6/30/08 |
| 8. QCS/QA Reviewer | Robert E. Spencer | Robert E Spencer | 6/30/08 |
| **APPROVAL** | | | |
| 9. Originator | Wendy A. Mitcheltree/David C. Sassani | Wendy Mitcheltree | 6/30/08 |
| 10. Responsible Manager | Paul R. Dixon | Paul R | 7-2-08 |

(Continued from Block 6)

This Error Resolution Document corrects errors in the document titled “In-Drift Precipitates/Salts Model”, ANL-EBS-MD-000045 Rev 03 based on evaluating the Audit Issues documented in CR 11102.

## I Background Information Summary

The condition description for CR 11102 is reproduced here as follows:

> CR Title: Audit Recommendations for ANL-EBS-MD-000045 Rev 03
>
> CR Description: Audit Issue #4 Recommend that CR discussions in AMRs provide more direct traceability to CR corrective actions. For example, reference the specific corrective action number that the AMR addresses.
>
> Audit Issue #20 CR 6731 is listed in Section 6.1 to be addressed in document ANL-EBS-MD-000045, Rev. 03, In-Drift Precipitates/Salts Model. This CR was not addressed in the document. It was determined that the CR was not pertinent to ANL-EBS-MD-000045, Rev. 03; therefore, it was removed from the planning document. Recommend that the discussion of CRs in AMRs match the intent of the technical work plans.
>
> Audit Issue #22 The Pitzer database used in the In Drift Precipitates/Salts Model is developed in Appendix I of ANL-EBS-MD-000045, Rev 03. Temperature limitations of the Pitzer database are clearly stated in Appendix I of ANL-EBS-MD-000045, Rev 03. The paragraph on page I-39 describing the temperature limitations states that, "Use of these parameters outside their respective ranges of validation is inadvisable and is not permitted for applications on the Yucca Mountain Project unless specific justification is provided." Section 7 provides a validation discussion which establishes the uncertainty of the IDPS Model including the uncertainty resulting from the temperature limitations of the Pitzer database. The final paragraph of Section 1 discusses the use of the Pitzer database with its inherent temperature limitations and the role of validation in determining that the model is valid for its intended use. However, it is unclear whether implicit justification for the use of the Pitzer database within the validation results constitutes specific justification as required for use of the database, per Appendix I. In addition, for complete documentation and clarity, the paragraph on page I-39 advising the user of the limited ranges of the Pitzer database should reference Table I-2 in addition to Table I-1 that is already referenced.
>
> Audit Issue #25 DTN: LL991008104241.042 is unqualified experimental data used as indirect input in Section 7.2.1 for validation. The traceability

from DTN: LL991008104241.042 to the scientific notebook SN-LLNL-SCI-372-V1 is difficult. Traceability would be improved if the comment block in the DTN coversheet was revised to include the full name of the notebooks with notes as to the experiments that are described in each notebooks and the cross references between the experiment names, C1, C2, C3 and the data sets corresponding to the experiments, evap1, evap2, evap4 that are actually used for the validation activities.

Audit Issue #30 Clarification regarding the first sentence of the 3rd full paragraph on page 7-93 beginning with, "It would be difficult to justify any model biases. . ." is necessary to understand its applicability to Figure 7-101 and the uncertainty ranges presented in Table 7-10. Though requirement 1 (above) was met, transparency referred to in requirement 2 (above) could be strengthened. Recommend explaining the limitations of the low relative humidity data on Figure 7-101 and how the data are used in the uncertainty ranges in Table 7-10.

Action 11102: Corrective Action Plan Summary

09/25/07 Robert E. Spencer - The recommendations (opportunities for improvement) taken from Audit # LLQA-IA-07-08 will be evaluated by Lead Lab management and addressed appropriately based on the evaluation. This plan includes one action for the applicable manager (or designee) to conduct the evaluation and identify the status of each of the recommendations (either the action to update ANL-EBS-MD-000045, Rev. 03, In-Drift Precipitates/Salts Model, or the justification as to why no action will be taken). This evaluation may take the form of a Word document, e-mail, etc. and will be attached to the CR as objective evidence for completion of the action.

The analysis below, in conjunction with files attached to the CR 11102, constitutes the evaluation referred to above.

## II Inputs and/or Software

No software or any types of calculations are used to evaluate the extent of condition in this CR. No assumptions were used in this analysis.

## III Analysis and Results

**Issue #4:** *(1) Traceability to CRs and related discussions in the report 'In-Drift Precipitates/Salts Model (ANL-EBS-MD-000045, REV 03)' are deemed as sufficient except for CR-6731. The latter is addressed by issue #20 below.*

No action needed for the IDPS AMR (ANL-EBS-MD-000045 REV 03) for this issue, except for CR-6731 as discussed in Issue #20 below. For changes regarding added traceability of CR-6731, see the section for Issue #20 below.

**Issue #4 Evaluation:** Traceability to CRs is sufficient in the report 'In-Drift Precipitates/Salts Model (ANL-EBS-MD-000045, REV 03)' except for CR-6731. Recommended actions for Issue #20 also related to CR-6731 are described below. Because there is no action here, there is no impact.

**Issue #20:** *(1) Traceability to CRs is sufficient in the report 'In-Drift Precipitates/Salts Model (ANL-EBS-MD-000045, REV 03)' except for CR-6731. This CR was mentioned but not addressed in the IDPS report. It was determined in the TWP of the IDPS AMR that CR-6731 was not relevant to the IDPS but a discussion of the disposition of CR-6731 should be added in the ERD text for added clarity on this issue. CR-6731 deals with discrepancies in the .thermodynamic data for phosphates.*

**Issue 20 Evaluation:** During the evaluation of this issue, it was determined that even though the IDPS report states in a number of places that the Pitzer database developed in Appendix I addressed the issue with the phosphate data corrections, the "readme.doc" file notes had not been added to indicate that the uncorrected phosphate data remained in the Pitzer datafile and that those data should not be used for quality affecting work. Because of this, a further evaluation of documents that utilized the Pitzer datafile has been completed and discussed below.

**Documents Evaluated for Impact of Using Pitzer Database (**SN0609T0502404.012. Pitzer Thermodynamic Database (DATA0.YP2)**)**

The DIRS reports for the documents below indicated the use of the Pitzer database (SN0609T0502404.012. Pitzer Thermodynamic Database (DATA0.YP2), Submittal date: 09/28/2006.) The usage and evaluation of impact are assessed below.

(1) MDL-NBS-HS-000001 Rev. 05 DRIFT-SCALE THC SEEPAGE MODEL:

**Evaluation**: The report used logK values from the Pitzer database. None of the minerals contain phosphate. Also the model used four starting pore water concentrations and none of them contained phosphate. Therefore, phosphate species from the database were not utilized within the simulations and thus there is no impact from the data on this downstream report.

(2) ANL-WIS-GS-000003 Rev. 01 QUALIFICATION OF THERMODYNAMIC DATA FOR GEOCHEMICAL MODELING OF MINERAL-WATER INTERACTIONS IN DILUTE SYSTEMS

**Evaluation**: The Pitzer Thermodynamic Database was used only as Indirect input (i.e., the uncorrected phosphate species were not used directly), so there is no impact from the data on this downstream report.

(3) TDR-TDIP-NF-000005 Rev. 00 TOTAL SYSTEM PERFORMANCE ASSESSMENT DATA INPUT PACKAGE FOR ENGINEERED BARRIER SYSTEM: PHYSICAL AND CHEMICAL ENVIRONMENT

**Evaluation**: The report used logK values from the Pitzer database. However, none of the input water compositions used in the simulations contained phosphate. Therefore, phosphate species from the database were not utilized within the simulations and thus there is no impact from the data on this downstream report.

(4) ANL-EBS-MD-000033 Rev. 06 ENGINEERED BARRIER SYSTEM: PHYSICAL AND CHEMICAL ENVIRONMENT

**Evaluation**: The report used logK values from the Pitzer database. However, none of the input water compositions used in the simulations contained phosphate. Therefore, phosphate species from the database were not utilized within the simulations and thus there is no impact from the data on this downstream report.

(5) TDR-WIS-PA-000014 Rev. 00 TSPA INFORMATION PACKAGE FOR THE DRAFT SEIS

**Evaluation**: The Pitzer Thermodynamic Database was used only as Indirect input (i.e., the uncorrected phosphate species were not used directly). The report discusses the use of EQ6 and the Pitzer database in conjunction with the PCE, which uses input waters without phosphate. There is no impact from the data on this downstream report.

(6) ANL-EBS-MD-000074 Rev. 01, Addendum 01 ANALYSIS OF DUST DELIQUESCENCE FOR FEP SCREENING

**Evaluation**: This report used the Pitzer database in simulations that included phosphate and therefore with the uncorrected logK values (output DTN: SN0706AMMONIUM.001). A detailed evaluation of the specific data and simulations analyzed in that output DTN was performed. It is concluded that there is no impact from the data on this downstream report or its conclusions as demonstrated in the detailed evaluation below.

***Detailed Evaluation of Using Pitzer Database (data0.yp2) in Dust Deliquescence AMR***

Section 6.7.8 of SNL 2007 [DIRS 177409] lists the phosphate corrections that were made to data0.ymp.R5 (the thermodynamic database for dilute solutions). Those corrections were not incorporated into the Pitzer database, data0.yp2 (DTN: SN0609T0502404.012 [DIRS 179067]). The Pitzer database was used as direct input for the evaporation

simulations documented in the *Analysis of Dust Deliquescence for FEP Screening* (SNL 2007 [DIRS 181267]), output DTN SN0706AMMONIUM.001. The phosphate corrections that were not included in the Pitzer database only apply to the simulations that include phosphate. Those sections of the addendum to the Dust Deliquescence AMR that used the uncorrected database are discussed below.

**Section 6.1.2.1[a], SNL 2007 [DIRS 181267]**
EQ6 simulations of cyclone dust leachate evaporation (containing phosphate), with ammonium present, that were performed using the Pitzer database were unsuccessful in determining the disposition of ammonium salt content. In the text (page 6-3) of the addendum (SNL 2007 [DIRS 181267]) and on the first page of the spreadsheet in the output DTN SN0706AMMONIUM.001 (*Cyclone dust ammonium partitioning.xls*) it is stated that the results were included in the output DTN, but were not used in other calculations. Since the results were not used in any further calculations and since the fact that the results were not used is well documented in the addendum and the output DTN, there is no impact from the data on this section of the downstream report.

**Section 6.1.2.2[a] and Section 6.1.2.3[a], SNL 2007 [DIRS 181267]**
The South Portal dust leachate compositions (containing phosphate, ammonium-modified) were evaporated using EQ6 and the Pitzer database. None of the EQ6 analyses reached a eutectic composition, and about half of them resulted in unreliable compositions. Other compositions may have been affected by a charge balancing issue (SNL 2007 [DIRS 181267], page 6-5. As a result, the South Portal dust leachate evaporation results were not included in the body of the report. The results were included in the output DTN, but were not used for other calculations.

The tunnel dust leachate compositions were ammonium-modified and evaporated using EQ3/6 and the Pitzer database. Those results are presented in Tables 6-3[a] and 6-4[a] of the addendum (SNL 2007 [DIRS 181267]).

For both the South Portal and the tunnel dust leachate samples, there was no impact in using the Pitzer database with the uncorrected phosphate data because:

1. **The differences in the logK values for the important phosphate reactions were very small.** The un-corrected logK values in the Pitzer database for the reactions of importance do not differ in any meaningful way (less than experimental uncertainties in general) from the corrected values in data0.ymp.R5 (DTN: SN0612T0502404.014 [DIRS 178850]), so the impact is negligible. The equations that control the phosphate in solution for these simulations are listed below in Table 1, along with the uncorrected values from the Pitzer database and the corrected logK values from data0.ymp.R5. There is no impact because the large magnitude of the logK values of fluorapatite compared to the difference is relatively minor.

Table 1. Comparison of logK values

| Reaction Equation | logK (25C) | |
|---|---|---|
| | data0.ymp.R5 | Pitzer data0.yp2 |
| Fluorapatite<br>Ca5(PO4)3F + 3H+ = 3HPO4-- + F- + 5Ca++ | -25.1410 | -24.9940 |
| H2PO4- = HPO4-- + H+ | -7.2120 | -7.2054 |
| PO4--- + H+ = HPO4-- | 12.3504 | 12.3218 |

Source: logK, data0.ymp.R5, from SNL 2007 [DIRS 177409], Tables 6-66, 6-72
logK, data0.yp2, from DTN: SN0609T0502404.012

2. **Minerals precipitated in the first step of the EQ6 simulations and did not dissolve throughout the simulation.** The output files from the EQ3 simulations indicate that the solutions were supersaturated with respect to fluorapatite ($Ca_5(PO_4)_3F$). (For example see DTN: SN0706AMMONIUM.001, file *EQ36 - NADP and (NH4)2SO4 adjusted\ Cyclone dusts_Summary_(NH4)2SO4_subtracted.xls* and file *Underground dusts_Summary_(NH4)2SO4_subtracted.xls*) . On the first EQ6 step of the simulations, fluorapatite precipitates. The quantity of the precipitated fluorapatite does not change during the evaporation simulation, showing that the mineral had no impact on the evaporation process. (For example see DTN: SN0706AMMONIUM.001, folder: *EQ36 - NADP and (NH4)2SO4 adjusted\ Cyclone dust\ Adj (NH4)2SO4 decomp* and folder *EQ36 - NADP and (NH4)2SO4 adjusted\ Underground dust\ Adj (NH4)2SO4 decomp*). The only exception was tunnel dust sample 574984, which showed a slight increase in mineral quantity, followed by a slight decrease. However because that sample is indicated to be contaminated it is not relevant (not used in the conclusions) and the slight variation is negligible (SNL 2007 [DIRS 181267], page 6-8).

3. **The presence of phosphate in the samples did not impact the results.** Phosphate does not have a big impact on the evaporation calculations, as demonstrated by comparing two tunnel dust samples (574982 and 574985), one which contains phosphate and one that does not. The resulting composition at the end of the evaporation, presented in Table 6-4[a], shows identical results. The results for the same two samples in Table 6-3[a] are not identical, but close enough to show that the presence of phosphate did not have any significant impact on the results. Because the presence or absence of phosphate did not have a significant impact on the evaporation results, then a slight variation in the logK of the phosphate equilibrium reactions would be expected to have a negligible impact. Even more important is that phosphate itself has no bearing on dust deliquescence and therefore the disparate values used in the analysis have no impact. Additionally, the impact is negligible when considering the use of the data within the dust deliquescence AMR. The three reactions using either databases are on the same magnitude and do not change the overall result (i.e., fluorapatite is still not soluble and the dissociation of H2PO4- and PO4- - - are of the same magnitude).

**Evaluation of Potential Impacts on Future use of Pitzer Database (data0.yp2) with uncorrected phosphate data**

A comparison was made between the phosphate corrections listed in Section 6.7.8 of SNL 2007 [DIRS 177409] and the logK values contained in the Pitzer database, DTN: SN0609T0502404.012 [DIRS 179067]. The Pitzer database does not contain all the reactions that are impacted by the phosphate corrections. The following table (Table 2) lists the aqueous species and solids that were corrected in data0.ymp.R5, but that remain uncorrected in the Pitzer database, data0.yp2. Table 2 also lists the type and qualitative magnitude on results of using the Pitzer database without implementing the corrections. The highlighted rows of Table 2 indicate the species for which some impact would be expected if the species were used within simulations. Assessment of the magnitude of those impacts is also given. For any future use of data0.yp2 this ERD (Table 2) should be consulted to determine appropriate use of the data. This was reiterated in readme for the Pitzer database DTN: SN0609T0502404.012 [DIRS 179067].

To address the above issues, the Appendix I of the IDPS AMR is corrected with the following statement (added as the last sentence of the first paragraph on page I-1):

> "Note that thermodynamic reaction properties data (i.e., not the Pitzer parameter values) for the phosphate species have not been corrected as indicated within CR 6731 and they are not updated in the manner done for the phosphate species in the dilute system database file data0.ymp.R5. Therefore, this Pitzer database should not be used for future simulations that include phosphate species without some further justification for intended usage of the specific data values included."

Also, as a result of this ERD, the following text was added to the "readme.doc" file of DTN: SN0609T0502404.012:

> "NOTE that thermodynamic reaction properties data for the phosphate system, (i.e., not the Pitzer parameter values), have not been updated in the manner of the data corrections for the phosphate species that were made in the dilute system database file data0.ymp.R5 (DTN: SN0702T0502404.015). This discrepancy was noted during corrective action for CR 11102. A discussion of the disparate values and the needed corrections to the text of the IDPS AMR are made within Model Error Resolution Document: ANL-EBS-MD-000045 ERD 02. This Pitzer database should not be used for future simulations that include phosphate species without some further justification for intended usage of the specific data values included."

**Issue #20 Evaluation Summary**: Although a number of documents (see list above) used the Pitzer database, only one used the uncorrected phosphate data in a direct manner (ANL-EBS-MD-000074 Rev. 01, Addendum 01). In that case, there were no impacts to the conclusions of the report because the simulations are not utilized further, and/or there was so little discrepancy in the values for the phosphate species included in the

simulations that there was negligible impact to the results from the presence of phosphate.

Given the above evaluations, the clarifying text for the IDPS AMR Appendix I (above), and the note added to the “readme.doc” file of the DTN: SN0609T0502404.012, there is no change to the conclusions of the IDPS AMR, nor impacts to any of the downstream reports, and therefore there is no impact from this issue and its corrections.

**Table 2. Future User Impact Evaluation of Using Pitzer Database with Uncorrected Phosphate data**

| Reaction Equation (containing 'PO4') | logK (25°C) | | Delta | Impact on using Pitzer |
|---|---|---|---|---|
| | data0.ymp.R5 | Pitzer data0.yp2 | | |
| ***Aqueous Species*** | | | | |
| HPO3-- + 0.5O2(g) = HPO4-- | 49.8056 | 48.6057 | 1.1999 | impact only for very reducing conditions (log fO2 <-48) |
| PO4--- + H+ = HPO4-- | 12.3504 | 12.3218 | 0.0286 | none |
| H2PO4- = HPO4-- + H+ | -7.2120 | -7.2054 | -0.0066 | none |
| H3PO4(aq) = HPO4-- + 2H+ | -9.3517 | -9.3751 | 0.0234 | none |
| AmH2PO4++ = HPO4-- + Am+++ + H+ | -10.2120 | -11.4119 | 1.1999 | small impact for solutions containing Am |
| ***Solids*** | | | | |
| Fluorapatite<br>Ca5(PO4)3F + 3H+ = 3HPO4-- + F- + 5Ca++ | -25.1410 | -24.9940 | -0.147 | none |
| Hydroxylapatite<br>Ca5(OH)(PO4)3 + 4H+ = 3HPO4-- + 5Ca++ + H2O | -8.4110 | -3.0746 | -5.3364 | higher solubility for systems without F, but no impact in systems with F because fluorapatite would form and be thermodynamically favored |
| Whitlockite<br>Ca3(PO4)2 + 2H+ = 2HPO4-- + 3Ca++ | -6.0658 | -4.2249 | -1.8409 | higher solubility for systems without F, but no impact in systems with F because fluorapatite would form and be thermodynamically favored |
| AmPO4(am) + H+ = Am+++ + HPO4-- | -12.4399 | -12.4683 | 0.0284 | none |
| Cu3(PO4)2 + 2H+ = 2HPO4-- + 3Cu++ | -12.1707 | -12.2247 | 0.054 | none |
| GdPO4:2H2O + H+ = HPO4-- + Gd+++ + 2H2O (data0.ymp.R5)<br>GdPO4:10H2O + H+ = HPO4-- + Gd+++ + 10H2O (data0.yp2) | -11.9495 | -11.9782 | 0.0287 | Pitzer has 10 H2O rather than 2; higher solubilities for concentrated solutions containing Gd |
| Co3(PO4)2 + 2H+ = 2HPO4-- + 3Co++ | -10.0036 | -10.0123 | 0.0087 | None |
| CoHPO4 = HPO4-- + Co++ | -6.7187 | -6.7223 | 0.0036 | None |
| NdPO4:H2O + H+ = HPO4-- + Nd+++ + H2O (data0.ymp.R5)<br>NdPO4:10H2O + H+ = HPO4-- + Nd+++ + 10H2O (data0.yp2) | -12.1495 | -12.1782 | 0.0287 | Pitzer 10 H2O rather than 1; higher solubilites for concentrated solutions containing Nd |
| Ni3(PO4)2 + 2H+ = 2HPO4-- + 3Ni++ | -4.2415 | -6.6414 | 2.3999 | lower solubility for solutions containing Ni |
| Pu(HPO4)2(am,hyd) = 2HPO4-- + Pu++++ | -30.4500 | -32.8499 | 2.3999 | lower solubility for solutions containing Pu |
| PuPO4(s,hyd) + H+ = HPO4-- + Pu+++ | -12.2500 | -13.4500 | 1.2 | lower solubility for solutions containing Pu |
| Th.75PO4 + H+ = HPO4-- + 0.75Th++++ | -15.6495 | -15.6782 | 0.0287 | none |
| U(HPO4)2:4H2O = 2HPO4-- + U++++ + 4H2O | -30.4577 | -32.8574 | 2.3997 | lower solubility for solutions containing U |
| UO2HPO4:4H2O = HPO4-- + UO2++ + 4H2O | -11.8123 | -13.0122 | 1.1999 | lower solubility for solutions containing U |

Source: logK, data0.ymp.R5, from SNL 2007 [DIRS 177409], Tables 6-66, 6-71, 6-72, 6-73, 6-75
logK, data0.yp2, from DTN: SN0609T0502404.012.

**Issue #22:** (1) *This issue pertains to the temperature limitations of the Pitzer database as stated in Appendix I of ANL-EBS-MD-000045 (Rev 03) and the paragraph on page I-39 with the statement "Use of these parameters outside their respective ranges of validation is inadvisable and is not permitted for applications on the Yucca Mountain Project unless specific justification is provided." The validation discussion in Section 7 of ANL-EBS-MD-000045 (Rev 03) establishes the uncertainty of the IDPS Model including the uncertainty resulting from the temperature limitations of the Pitzer database. The issue lies on whether justification and use of the Pitzer database in the IDPS model validation allows for the intended use of the data given its inherent limitations in terms of temperature applicability range, for example. It's also been suggested to add pointers to Tables I-1 and I-2 to advise the user of the limitation on temperature ranges of the Pitzer database.*

**Issue #22 Evaluation:** The retrieval of Pitzer parameter data is based on data with limits on salt concentrations (i.e., ionic strength) and temperature. These limits defined the applicability range of the data for a given chemical system. The cautionary note identified below is intended to highlight these limitations which are common to all thermodynamic databases. The validation activities in ANL-EBS-MD-000045 (Rev 03) should be viewed as independent tests of the predictive capabilities of the code and the Pitzer parameter data for a given salt system and temperature conditions. If some of these cases exceed the stated limits but the predictions still met the model validation criteria, then this should be viewed in and of itself as the additional specific justification for using the data. None of these clarifications impact the conclusions of the IDPS model report and do not impact any of the usages of the model.

The relevant text in paragraph on page I-39 of Appendix I in ANL-EBS-MD-000045 (Rev 03) has been rewritten (see below) to clearly state that the cautionary note about the Pitzer database usage is intended to be general as with the use of any other thermodynamic database in geochemical modeling. The relevant text is corrected to read as follows (cautionary note):

"The user is advised of the limited ranges listed in Tables I-1 and I-2 for several Pitzer parameters. The user must consult the original sources for more information on the permissible physico-chemical conditions for which the parameter data are qualified. Use of these parameter data outside their respective qualification ranges is inadvisable and is not permitted for applications on the Yucca Mountain Project unless specific justification is provided. The validation activities and criteria of the IDPS model serve as specific justification for such intended usage of the data."

None of these clarifications impact the conclusions of the IDPS model report and do not impact any of the usages of the model.

**Issue #25**: *This issue is related to the use of the unqualified DTN: LL991008104241.042 that contains experimental data utilized as indirect input in Section 7.2.1. This DTN is traced to the scientific notebook SN-LLNL-SCI-372-V1 but data traceability within this document is difficult.*

**Issue #25 Evaluation:** Overall traceability of data DTN: LL991008104241.042 in the scientific notebook SN-LLNL-SCI-372-V1 is difficult but sufficient. No action is needed on the AMR because this is a recommendation for clearer traceability in a scientific notebook. Therefore, no corrections are made to the IDPS AMR to address this issue. This does not impact any aspect of the conclusions of the IDPS model report and the scientific notebook does not require clarification.

**Issue #30:** *(1) This issue relates to statements in the 3rd paragraph on page 7-93 regarding the quantification of model biases and how clear these are delineated in figures 7-101 and Table*
*7-10. It is recommended to expand the explanation on the limitations inherent to low relative humidity data on Figure 7-101 and how these data are used in defining the uncertainty ranges in Table 7-10.*

**Issue #30 Evaluation:** The 3rd paragraph on page 7-93 of in ANL-EBS-MD-000045 (Rev 03) provides sufficient explanations concerning the limitations on data availability for some salt systems and the difficulties in quantifying biases given the unequal population of data at certain relative humidities (RHs). Moreover, the experimental error on these data is not directly quantified. Therefore, all potential errors, including estimated experimental errors and those related to inherent complexities in the modeling of multi-component salt systems, are captured in the uncertainty estimate presented in Table 7-10. This approach is considered adequate until more data and related uncertainties become available for the salt systems in question, especially at the physico-chemical conditions expected in the repository. There are no changes made to the IDPS AMR for this issue. There is no impact to any of the conclusions of the IDPS model report.

## IV Impact Evaluation and Summary

Based on addressing CR 11102, there is no impact to the conclusions or the results of the In-Drift Precipitates/Salts Model (ANL-EBS-MD-000045 Rev 03). None of the downstream documents using the results of this IDPS document are impacted in any manner.

The following is a list of documents that use ANL-EBS-MD-000045 Rev03 (DIRS# 177411) as a source: ANL-EBS-MD-000033 Rev. 06, ANL-EBS-MD-000074 Rev. 01, Addendum 01, ANL-EBS-MD-000037 Rev. 04, Addendum 01, ANL-WIS-GS-000003 Rev. 01, ANL-WIS-MD-000024 Rev. 01, ANL-WIS-MD-000027 Rev. 00, MDL-NBS-HS-000001 Rev. 05, MDL-WIS-PA-000005 Rev. 00, and TDR-WIS-PA-000014 Rev. 00. Also, in all cases ANL-EBS-MD-000045 Rev03 (DIRS# 177411) was used as Indirect Input.