Appendix B

NUCLEAR WASTE MANAGEMENT PROCEDURE — Sandia National Laboratories	**Parameter Problem Report (PPR)**	**Form Number: NP 9-2-2** **Page 1 of 1**

Material Abbreviated Name: SOLMOD5

Property Abbreviated Name: SOLSOH

Associated Analysis: (CCA, PAVT, AP-159, etc.) CRA19

Effective Date: 4/16/2019

Description of Problem

The beta(0) term for the binary Pitzer parameter for Ca2+ / EDTA4- pair was entered incorrectly in the EQ3/6 thermodynamic database DATA0.FM4. It was entered as 5.39 when the correct value is 2.48. While this value is NOT a direct input to PA, it could have had a tertiary impact on the SOLMOD5 parameter value.

Paul Domski 11/13/19
Requester (Print, Sign and Date)

Condition Adverse to Quality? ☐ Yes ☒ No (Initiate NP 16 –1 if yes)

Problem Resolution and Justification for no Condition Adverse to Quality

An analysis memo ("Correction of a Binary Pitzer Parameter in DATA0.FM4, PPR 2019-003") was created to determine if the incorrect Pitzer parameter value had an adverse effect on quality, and the results showed that it did not. Therefore, the parameter is unchanged and will not be changed in the PAPDB.

To help prevent a similar error from reoccurring, a statement will be added to the opening comments of all future WIPP EQ3/6 thermodynamic databases which reads: "NOTICE: When adding new data blocks, or modifying existing data blocks ALWAYS use the original reference to insure the correct parameter values are being included." A set of "lesson-learned" slides was prepared and distributed to the technical staff with active QA training to further avoid this from reocurring.

Concurrence

PAUL E. SHOEMAKER 11/14/19
PA Manager (Print, Sign and Date)

SHELLY R. NIELSEN 11-13-19
QA Staff (Print, Sign and Date)

2019-003
Parameter Problem Report No. (PPR)

Information Only

Triventi, Antonio

From:	Domski, Paul S
Sent:	Wednesday, November 13, 2019 11:07 AM
To:	Sisk-Scott, Charlotte; Jang, Jay Je-Hun; Zhang, Luzheng; Kirkes, Leslie; Kim, Sungtae
Cc:	Triventi, Antonio; Nielsen, Shelly R; Long, Jennifer J
Subject:	Lessons Learned: Error found in the WIPP Pitzer Thermodynamic Database
Attachments:	FM4_Lessons_DATA0.FM4.pptx

Dear Colleagues,

Attached you will find a short Powerpoint presentation that I put together to help the Geochemistry team avoid future errors in the creation of Pitzer Thermodynamic databases, and any other documents or databases which require the transcription of a large number of numerical values. Please take a few minutes to read over the presentation and think about how it may apply to your work. If you have any questions or comments please feel free to contact me. Thank you.

P.S. Feel free to distribute this to anyone to whom this may benefit.

Paul Domski
(505) 604-6736

Information Only

Sandia National Laboratories

Lessons Learned:

Error found in the WIPP Pitzer Thermodynamic Database





PRESENTED BY

Paul S. Domski

ENERGY NNSA

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Information Only

The Problem

An incorrect value for the binary Pitzer parameter $\beta^{(0)}$ for the Ca^{2+} /$EDTA^{4-}$ was entered in the DATA0.FM4 EQ3/6 Pitzer thermodynamic database. This database functions as the official WIPP QA Pitzer Thermodynamic Database for use quality affecting work.

Information Only

Why this happened

1. In order to meet project deadlines under a heavy workload the Geochemistry team was required to re-evaluate previously established parameters for the Pitzer thermodynamic database. As such, not enough time existed to reveal any potential errors by completing extensive testing prior to deem the WIPP Pitzer thermodynamic database "ready-for-use".
2. PA calculations are typically the culmination of work that originates from many investigators who work independently, and, as such, a lot comes down to the wire with the associated risk of being delivered as "disjoint" work.
3. Intense workload, and, as such, increased risk for inattention to details and for shortcuts.

Information Only

What were the lessons learned?

1. Every effort should be made to ensure the WIPP Pitzer thermodynamic database is "ready-for-use" months ahead of an expected PA calculation. A better coordination in setting PA deadlines and timelines according to Geochemistry workload would provide an opportunity to take into consideration the time needed for extensive testing of the database.
2. Every effort should be made to ensure work is appropriately evaluated and not being done in parallel if the risk of creating a condition adverse to quality by delivering "disjoint" work exist.
3. Every effort should be made to ensure investigators work from the most recent, final, and original references when creating downstream documents such as databases and reports. Investigators should embrace the practice of having multiple eyes on their work by asking colleagues, outside of the official WIPP QA review process, to go over technical elements including numbers and equations. Remember, the more people who look at your work, the fewer chances there are for errors.

Information Only