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Sandia National Laboratories
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Carlsbad, New Mexico 88220

Date: January 9, 2020

To: SNL WIPP Records Center
Defense Waste Management Programs Group

From: Paul S. Domski, MS (Org. 08882) Shelly R. Nielsen for

Subject: Correction of the α_1 terms of three Binary Pitzer Parameter blocks in DATA0.FM4, PPR 2019-004 through 2019-013.

The α_1 terms for the binary Pitzer parameter blocks for Ca^{2+} / $EDTA^{4-}$, Mg^{2+} / $MgEDTA^{2-}$, and the Ca^{2+} / $MgEDTA^{2-}$ pairs were entered incorrectly in the EQ3/6 thermodynamic database DATA0.FM4. They were entered as 2.0 when the correct value is 1.4 (Jang, 2019). This issue was uncovered during an extent of condition evaluation triggered by Parameter Problem Reports (PPR) 2019-003 (Domski, 2019a and 2019b). While these α_1 terms are NOT direct inputs to PA, they did impact the Actinide (An)(III) material property (SOLMOD3) PA parameter for both the Salado brine (GWB) and Castile brine (ERDA-6), at the five brine volumes (Property SOLSOH – SOLSOH5 and SOLCOH – SOLCOH5, respectively). This fact alone does not constitute a condition adverse to quality, rather, only if the models that use these parameters as input are impacted negatively would this be considered a condition adverse to quality.

The α_1 values for all of the binary Pitzer parameter blocks included in DATA0.FM4 were checked to insure the correct values were used, and no other errors were found. The extent of this condition was limited to the Ca^{2+} / $EDTA^{4-}$, Mg^{2+} / $MgEDTA^{2-}$, and the Ca^{2+} / $MgEDTA^{2-}$ binary Pitzer data blocks, no other data blocks were impacted. PPR's 2019-004 through 2019-013 (Domski, 2019b) were initiated per NP 9-2 Revision 2 Section 2.5 with the discovery of the incorrect α_1 terms for the binary Pitzer parameter blocks. This memorandum functions as the documentation for the PPR resolution and serves as justification for why the issue did not lead to a condition adverse to quality.

To determine if α_1 terms had an impact on the CRA-2019 PA baseline solubility model, a copy of the interim database DATA0.F4F, created from DATA0.FM4 and documented in Domski (2019a), was made and renamed DATA0.F5F, with DATA0.F5F being the name of the database with the α_1 terms updated to the correct values. See Appendix I for the updated binary Pitzer blocks used in DATA0.F5F. The database, DATA0.F5F, was then used to run the baseline solubility model 1x through 5x volumes cases for GWB and ERDA-6, and the results were compared to those documented in Tables 6 and 7 in Domski and Sisk-Scott (2019). The database DATA0.F5F was created for scoping purposes and did not require WIPP SNL Quality Assurance documentation.

The results showed that there were changes to the Am(III) concentrations for both brines at the five dilutions compared to the concentrations in Domski and Sisk-Scott (2019). This was determined by extracting the results calculated by both databases in Excel using the macro GetEQdata.xlsx and

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comparing the results with Tables 6 and 7 for GWB and ERDA-6, respectively, from Domski and Sisk-Scott (2019a). All files can be found in the CMS:
/nfs/data/CVSLIB/WIPP_EXTERNAL/ap183_database correction

Tables 1 and 2 provide the results of the comparison of DATA0.FM4 with DATA0.F5F, for GWB and ERDA-6, respectively. The results show that only the Am(III) concentrations change using the DATA0.F5F database, and that the remainder of the other concentrations and solution properties remain the same.

Table 1. Comparison of EQ3/6 Predictions of the Compositions and Solubilities of Th(IV), Np(V), and Am(III) in Five Different Volumes of GWB (M (molarity) Unless Otherwise Noted) between DATA0.FM4 and DATA0.F5F.

Element or Property	1 × Minimum[A] DATA0.FM4	1 × Minimum DATA0.F5F	2 × Minimum DATA0.FM4	2 × Minimum DATA0.F5F	3 × Minimum DATA0.FM4	3 × Minimum DATA0.F5F
B(III)(aq)	0.224	0.224	0.231	0.231	0.233	0.233
Na(I)(aq)	4.69	4.69	4.71	4.71	4.71	4.71
Mg(II)(aq)	0.348	0.348	0.336	0.336	0.332	0.332
K(I)(aq)	0.663	0.663	0.682	0.682	0.688	0.688
Ca(II)(aq)	1.09E-02	1.09E-02	1.07E-02	1.07E-02	1.06E-02	1.06E-02
Fe(II)(aq)	2.61E-05	2.61E-05	2.61E-05	2.61E-05	2.60E-05	2.60E-05
S(VI)(aq)	0.232	0.232	0.233	0.233	0.234	0.234
Cl(-I)(aq)	5.40	5.40	5.43	5.43	5.43	5.43
Br(-I)(aq)	3.78E-02	3.78E-02	3.88E-02	3.88E-02	3.92E-02	3.92E-02
Pb(II)(aq)	1.90E-02	1.90E-02	1.90E-02	1.90E-02	1.90E-02	1.90E-02
Th(IV)(aq)	5.45E-08	5.45E-08	5.45E-08	5.45E-08	5.45E-08	5.45E-08
Np(V)(aq)	4.02E-07	4.02E-07	2.83E-07	2.83E-07	2.42E-07	2.42E-07
Am(III)(aq)	**1.63E-07**	**1.66E-07**	**1.58E-07**	**1.59E-07**	**1.56E-07**	**1.57E-07**
f_{CO_2} (atm)	2.02E-06	2.02E-06	2.02E-06	2.02E-06	2.02E-06	2.02E-06
I	6.53	6.53	6.55	6.55	6.55	6.55
pH[B]	8.82	8.82	8.82	8.82	8.82	8.82
pcH	9.54	9.54	9.55	9.55	9.55	9.55
RH (%)[C]	73.2	73.2	73.2	73.2	73.2	73.2
TIC[D]	2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04

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Table 1. Comparison of EQ3/6 Predictions of the Compositions and Solubilities of Th(IV), Np(V), and Am(III) in Five Different Volumes of GWB (M (molarity) Unless Otherwise Noted) between DATA0.FM4 and DATA0.F5F (continued).

Element or Property	4 × Minimum DATA0.FM4	4 × Minimum DATA0.F5F	5 × Minimum DATA0.FM4	5 × Minimum DATA0.F5F
B(III)(aq)	0.234	0.234	0.235	0.235
Na(I)(aq)	4.71	4.71	4.71	4.71
Mg(II)(aq)	0.330	0.330	0.329	0.329
K(I)(aq)	0.692	0.692	0.694	0.694
Ca(II)(aq)	1.06E-02	1.06E-02	1.05E-02	1.05E-02
Fe(II)(aq)	2.60E-05	2.60E-05	2.60E-05	2.60E-05
S(VI)(aq)	0.234	0.234	0.234	0.234
Cl(-I)(aq)	5.44	5.44	5.44	5.44
Br(-I)(aq)	3.94E-02	3.94E-02	3.95E-02	3.95E-02
Pb(II)(aq)	1.91E-02	1.91E-02	1.91E-02	1.91E-02
Th(IV)(aq)	5.45E-08	5.45E-08	5.45E-08	5.45E-08
Np(V)(aq)	2.21E-07	2.21E-07	2.09E-07	2.09E-07
Am(III)(aq)	**1.55E-07**	**1.56E-07**	**1.54E-07**	**1.55E-07**
f_{CO_2} (atm)	2.02E-06	2.02E-06	2.02E-06	2.02E-06
I	6.55	6.55	6.55	6.55
pH[B]	8.82	8.82	8.82	8.82
pcH	9.55	9.55	9.55	9.55
RH (%)[C]	73.2	73.2	73.2	73.2
TIC[D]	2.50E-04	2.50E-04	2.50E-04	2.50E-04

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Table 2. Comparison of EQ3/6 Predictions of the Compositions and Solubilities of Th(IV), Np(V), and Am(III) in Five Different Volumes of ERDA-6 (M (molarity) Unless Otherwise Noted) between DATA0.FM4 and DATA0.F5F.

Element or Property	1 × Minimum[A] DATA0.FM4	1 × Minimum DATA0.F5F	2 × Minimum DATA0.FM4	2 × Minimum DATA0.F5F	3 × Minimum DATA0.FM4	3 × Minimum DATA0.F5F
B(III)(aq)	0.281	0.281	0.282	0.282	0.282	0.282
Na(I)(aq)	4.66	4.66	4.70	4.70	4.72	4.72
Mg(II)(aq)	0.435	0.435	0.391	0.391	0.374	0.374
K(I)(aq)	0.499	0.499	0.563	0.563	0.590	0.590
Ca(II)(aq)	1.28E-02	1.28E-02	1.19E-02	1.19E-02	1.16E-02	1.16E-02
Fe(II)(aq)	2.67E-05	2.67E-05	2.64E-05	2.64E-05	2.64E-05	2.64E-05
S(VI)(aq)	0.224	0.224	0.228	0.228	0.229	0.229
Cl(-I)(aq)	5.22	5.22	5.29	5.29	5.32	5.32
Br(-I)(aq)	5.66E-02	5.66E-02	6.39E-02	6.39E-02	6.69E-02	6.69E-02
Pb(II)(aq)	1.88E-02	1.88E-02	1.90E-02	1.90E-02	1.90E-02	1.90E-02
Th(IV)(aq)	5.44E-08	5.44E-08	5.44E-08	5.44E-08	5.44E-08	5.44E-08
Np(V)(aq)	1.20E-06	1.20E-06	7.27E-07	7.27E-07	5.52E-07	5.52E-07
Am(III)(aq)	**1.78E-07**	**1.90E-07**	**1.63E-07**	**1.70E-07**	**1.58E-07**	**1.62E-07**
f_{CO_2} (atm)	2.02E-06	2.02E-06	2.02E-06	2.02E-06	2.02E-06	2.02E-06
I	6.48	6.48	6.52	6.52	6.53	6.53
pH[B]	8.82	8.82	8.82	8.82	8.82	8.82
pcH	9.52	9.52	9.53	9.53	9.53	9.53
RH (%)[C]	73.2	73.2	73.2	73.2	73.2	73.2
TIC[D]	2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04

Table 2. Comparison of EQ3/6 Predictions of the Compositions and Solubilities of Th(IV), Np(V), and Am(III) in Five Different Volumes of ERDA-6 (M (molarity) Unless Otherwise Noted) between DATA0.FM4 and DATA0.F5F (continued).

Element or Property	4 × Minimum DATA0.FM4	4 × Minimum DATA0.F5F	5 × Minimum DATA0.FM4	5 × Minimum DATA0.F5F
B(III)(aq)	0.282	0.282	0.283	0.283
Na(I)(aq)	4.72	4.72	4.73	4.73
Mg(II)(aq)	0.365	0.365	0.360	0.360
K(I)(aq)	0.604	0.604	0.612	0.612
Ca(II)(aq)	1.14E-02	1.14E-02	1.13E-02	1.13E-02
Fe(II)(aq)	2.63E-05	2.63E-05	2.63E-05	2.63E-05
S(VI)(aq)	0.230	0.230	0.231	0.231
Cl(-I)(aq)	5.34	5.34	5.35	5.35

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Br(-I)(aq)	6.84E-02	6.84E-02	6.94E-02	6.94E-02
Pb(II)(aq)	1.90E-02	1.90E-02	1.91E-02	1.91E-02
Th(IV)(aq)	5.44E-08	5.44E-08	5.44E-08	5.44E-08
Np(V)(aq)	4.61E-07	4.61E-07	4.05E-07	4.05E-07
Am(III)(aq)	**1.54E-07**	**1.58E-07**	**1.52E-07**	**1.55E-07**
f_{CO_2} (atm)	2.02E-06	2.02E-06	2.02E-06	2.02E-06
I	6.54	6.54	6.55	6.55
pH[B]	8.82	8.82	8.82	8.82
pcH	9.54	9.54	9.54	9.54
RH (%)[C]	73.2	73.2	73.2	73.2
TIC[D]	2.50E-04	2.50E-04	2.50E-04	2.50E-04

Footnotes for Tables 1 and 2:

A. Based on a minimum brine volume of 17,400 m^3 (Clayton, 2008)
B. The Pitzer scale is an unofficial pH scale consistent with pH values calculated using single-ion activity coefficients based on the Pitzer activity-coefficient model for brines and evaporite minerals of Harvie et al. (1984), extended to include Nd(III), Am(III), and Cm(III); Th(IV); and Np(V). T. J. Wolery of Lawrence Livermore National Laboratory (LLNL) in Livermore, CA, proposed the term "Pitzer scale" unofficially.
C. RH = Relative Humidity. The value of the RH divided by 100 yields the value of the activity of H_2O in GWB and ERDA-6.
D. TIC = Total Inorganic C.

Tables 3 and 4 provide the Salado (GWB) and Castile (ERDA-6) SOLMOD3 parameter comparisons for the five volume cases.

Table 3. Salado (GWB) SOLMOD3 Parameter Comparison.

Database	Am(III) Molarity	Material	Property
DATA0.FM4	1.63E-07	SOLMOD3	SOLSOH
DATA0.F5F	1.66E-07	SOLMOD3	SOLSOH
DATA0.FM4	1.58E-07	SOLMOD3	SOLSOH2
DATA0.F5F	1.59E-07	SOLMOD3	SOLSOH2
DATA0.FM4	1.56E-07	SOLMOD3	SOLSOH3
DATA0.F5F	1.57E-07	SOLMOD3	SOLSOH3
DATA0.FM4	1.55E-07	SOLMOD3	SOLSOH4
DATA0.F5F	1.56E-07	SOLMOD3	SOLSOH4
DATA0.FM4	1.54E-07	SOLMOD3	SOLSOH5
DATA0.F5F	1.55E-07	SOLMOD3	SOLSOH5

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Table 4. Castile (ERDA-6) SOLMOD3 Parameter Comparison.

Database	Am(III) Molarity	Material	Property
DATA0.FM4	1.78E-07	SOLMOD3	SOLCOH
DATA0.F5F	1.90E-07	SOLMOD3	SOLCOH
DATA0.FM4	1.63E-07	SOLMOD3	SOLCOH2
DATA0.F5F	1.70E-07	SOLMOD3	SOLCOH2
DATA0.FM4	1.58E-07	SOLMOD3	SOLCOH3
DATA0.F5F	1.62E-07	SOLMOD3	SOLCOH3
DATA0.FM4	1.54E-07	SOLMOD3	SOLCOH4
DATA0.F5F	1.58E-07	SOLMOD3	SOLCOH4
DATA0.FM4	1.52E-07	SOLMOD3	SOLCOH5
DATA0.F5F	1.55E-07	SOLMOD3	SOLCOH5

The PA material parameter SOLMOD3 represents the Am(III) total concentration for GWB and ERDA-6 at the five brine volumes (Property SOLSOH – SOLSOH5 and SOLCOH – SOLCOH5, respectively) as predicted by the baseline solubility model (Domski and Sisk-Scott, 2019). The Am(III) concentration at two volumes, the 1x and 5x volumes (SOLSOH and SOLSOH5, and SOLCOH and SOLCOH5), are used by the humic colloids model to calculate the PA parameters PHUSIM and PHUCIM (Mariner, 2019), which are PA input parameters. Therefore, an assessment was made by Mariner (see e-mail correspondence Appendix II) to determine if PHUSIM and PHUCIM were affected by these changes to the Am(III) concentrations. Mariner determined that the changes to the Am(III) concentrations caused by the updated α_1 terms for the binary Pitzer parameter blocks did not change the values of PHUCIM and PHUSIM (see Appendix II). Therefore, there is no condition adverse to quality with regard to these humic colloid PA parameters, and the PHUSIM and PHUCIM parameters will not be updated in the WIPP PA Parameter Database.

Kim (2019) examined the effect of the changes to the SOLMOD3 parameter on the mobilized An(III) concentration, the repository brine pressure, the hydrogen gas generation rate, and the total An(III) release to the Culebra Formation for CRA-2019 Deferred PA. Kim accomplished this by using the updated SOLMOD3 parameters which resulted from DATA0.F5F, and the running the PA code to determine if the total release CCDFGF curve was changed relative to the CCDFGF curve using the SOLMOD3 parameters from DATA0.FM4. Kim (2019) concluded: "The parameters will not be updated in the WIPP PA Parameter Database as this analysis results have demonstrated that there is no impact caused by the error that created the slight changes in the SOLMOD3 parameter values.", and "…the SOLMOD3 material property parameter updates did not impact the Total Release and its CCDFGF curve. In other words, the α_1 terms included in the Pitzer thermodynamic database, DATA0.FM4, did not result in a condition adverse to quality with regard to the CRA-2019 Deferred PA.

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Conclusions

This memo serves as documentation for Problem Parameter Reports (PPR) 2019-004 2019-013 that were initiated per NP 9-2 Revision 2 Section 2.5. While it was shown that the PA material parameter SOLMOD3 was affected by errors in the DATA0.FM4 database, it was also shown that the "downstream" impact of these errors was not adverse to quality. Therefore, no further action is required as this memo and the PPR's 2019-004 through 2019-013 are records that there was no impact to quality, and PHUSUM, PHUCIM, and the SOLMOD3 parameters will not be updated in the WIPP PA Parameter Database.

A QA version of the WIPP Pitzer thermodynamic database, DATA0.FM5, has been created from the interim database, DATA0.F5f, that includes the corrected value of the binary Pitzer parameter block for Ca^{2+} / $EDTA^{4-}$, $\beta^{(0)} = 2.48$ (Domski, 2019a), as well as the corrected α_1 terms for the binary Pitzer parameter blocks for Ca^{2+} / $EDTA^{4-}$, Mg^{2+} / $MgEDTA^{2-}$, and the Ca^{2+} / $MgEDTA^{2-}$ pairs. Release of DATA0.FM5 is contingent upon this PPR memo and the PPR forms being entered into the official WIPP records center.

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REFERENCES

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Domski, P.S. 2019. "Official Release of the Qualified Pitzer Thermodynamic Database, DATA0.FM4, for EQ3/6 under AP-183, Revision 1. Carlsbad, NM: Sandia National Laboratories. ERMS# 571051.

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Jang, J-H. 2019. "Analysis Plan for Derivation and Addition of Equilibrium Constants and Pitzer Interaction Parameters to the WIPP Geochemical Thermodynamic Database". AP-182 (2019). Carlsbad, NM: Sandia National Laboratories. ERMS# 571074.

Kim, S. 2019. "Impact Analysis of Corrected Actinide (III) Baseline Solubility Parameters on Performance Assessments". Carlsbad, NM: Sandia National Laboratories. (ERMS# not yet issued).

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Nuclear Waste Management Procedure NP 9-2, Parameters Revision 2. April 25, 2017. Carlsbad, NM: Sandia National Laboratories.

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SNL/WIPP Records Center (to be included in the AP-183 records package)

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Appendix I.

```
+--------------------------------------------------------------------
Ca++                          EDTA----
  alpha(1) = 1.4
  alpha(2) = 12.0
  beta(0)
    a1 = 2.48
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Domski(2018)
+--------------------------------------------------------------------
Mg++                          CaEDTA--
  alpha(1) = 1.4
  alpha(2) = 12.0
  beta(0)
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 7.21
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Domski(2018)
+--------------------------------------------------------------------
Mg++                          MgEDTA--
  alpha(1) = 1.4
  alpha(2) = 12.0
  beta(0)
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 7.27
```


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```
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Domski(2018)
+---------------------------------------------------------------------
```


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Appendix II.

From: Mariner, Paul
Sent: Thursday, November 14, 2019 2:45 PM
To: Domski, Paul S
Subject: RE: DATA0.FM4

Hi Paul,

Because the log K values were not affected, these changes didn't affect any of the PHREEQC calculations. The hand calculations (done with Mathcad) were only affected for An(III), but changes were negligible. New calculations for An(III) are slightly less than before (no more than 6% less), but rounding gives the same An(III) PHUMSIM and PHUMCIM values recommended for CRA-2019: 0.2 for each of them.

- Paul

From: Domski, Paul S
Sent: Wednesday, November 13, 2019 2:57 PM
To: Mariner, Paul <pmarine@sandia.gov>
Subject: Re: DATA0.FM4

Here's the database, for the time being it's being called DATA0.F5F, the first three Pitzer blocks at the top of the database, Ca2+/EDTA4-, Ca2+/MgEDTA2-, and Mg2+/MgEDTA2- were the ones that were corrected. They all had the wrong alpha(0)[1] values, and beta(0) for Ca2+/EDTA4- was also wrong.

I'll send the brine compositions in a minute.

Paul Domski
(505) 604-6736

From: Mariner, Paul
Sent: Wednesday, November 13, 2019 2:44 PM
To: Domski, Paul S
Subject: RE: DATA0.FM4

Paul,

Please send me the new EDTA reactions in FM5 data0 (any other new reactions?). I use them when I derive the Am-humic and Th-humic log K values.

Also, do you have new 1x and 5x equilibrated compositions for GWB and ERDA-6? I use several chemical parameters from them (e.g., pH, free Am+3, free Ca+2, etc.) to estimate PHUMSIM and PHUMCIM, prior to rounding up.

[1] Note: In the email by Domski it states "alpha(0)", it should have been written as "alpha(1)".

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Thanks
- Paul

From: Domski, Paul S
Sent: Wednesday, November 13, 2019 12:02 PM
To: Mariner, Paul <pmarine@sandia.gov>
Cc: Sisk-Scott, Charlotte <csisksc@sandia.gov>; Nielsen, Shelly R <srjohn@sandia.gov>
Subject: Re: DATA0.FM4

Thanks Paul, much appreciated.

Paul Domski
(505) 604-6736

From: Mariner, Paul
Sent: Wednesday, November 13, 2019 11:58 AM
To: Domski, Paul S
Subject: RE: DATA0.FM4

Ok I will try in the next day or so. I just returned to work and have several things on my plate. My guess is that this change won't have an effect because of some built-in safety factors, but we won't know until I work through the calculations.

- Paul

From: Domski, Paul S
Sent: Wednesday, November 13, 2019 11:54 AM
To: Mariner, Paul <pmarine@sandia.gov>
Subject: Re: DATA0.FM4

As soon as is feasible. We are in the process of writing up Parameter Problem Reports via NP 9-2, and we need to know if this problem will impact PHUCIM and PHUSIM, I think are the variable names.

Paul Domski
(505) 604-6736

From: Mariner, Paul
Sent: Wednesday, November 13, 2019 11:49 AM
To: Domski, Paul S
Subject: RE: DATA0.FM4

Hi Paul. I can look into this. How soon do you need an answer?
- Paul

From: Domski, Paul S
Sent: Tuesday, November 12, 2019 12:52 PM

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To: Mariner, Paul <pmarine@sandia.gov>
Subject: DATA0.FM4

Hi Paul,

I hope you are well. We have found an error in DATA0.FM4 in three of the binary Pitzer parameter pairs, Ca2+ / EDTA4-, Mg2+ / MgEDTA2-, and Mg2+ / CaEDTA2-. I have re-run the baseline solubility model and the only thing that changes is a slight increase in the total Am(III) concentration. See the attached document, the bold values are the corrected concentrations for the two brines at increasing dilutions. Please let me know if you think this will impact your model. Thank you.

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Information Only