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to: SNL WIPP Records Center
Defense Waste Management Programs

from: Paul S. Domski Shelby R. Nielsen for

subject: Memo AP-173, EQ3/6 Database Update: DATA0.FM2

This memo documents the steps used to create a quality assured thermodynamic database, DATA0.FM2, in accordance with AP-173 revision 1(Domski and Xiong 2015). The steps are as follows:

1) Copy DATA0.FM1 (Xiong 2011) to DATA0.FM2.
2) Edit DATA0.FM2 and enter all of the fitting and supporting parameters from AP-154, revision 2 (Xiong 2013), AP-155, revision 3 (Xiong 2014), and AP-173, revision 1 as listed in AP-173. Note the analysis plans will be called AP-154, AP-155, and AP-173 without their revision numbers for the remainder of this document.
3) Run the parameter fitting Python scripts using DATA0.FM2 for each of the tasks listed in AP-173.
4) Compare the results with those documented in the analysis reports, and memos, i.e., the original derived parameter values. The original derived values (documented value) were accepted if the results of fitting with DATA0.FM2 were within 10% of the value, which is a deviation from acceptance criteria of AP-173. It was expected that there would be some deviation between the original derived values and those derived with DATA0.FM2 because of the necessity of deriving the parameters in a stepwise fashion.
5) If the difference in the fitted parameter values using DATA0.FM2 was greater than 10%, then the appropriate analysis report, or memo, was updated to reflect the new parameters and DATA0.FM2 was also updated to reflect these changes.

Tables 1, 2, and 3 list the tasks and parameters for AP-154, AP-155, and AP-173, respectively, and compares the values documented in the analysis reports, and memos, in the table column labeled "Documented Value", with those estimated using the new database DATA0.FM2. A complete listing of the parameter blocks, both fitting and supporting data, that were added to DATA0.FM1 is provided in Appendix A.

Note that the $\beta^{(1)}$ and C^{ϕ} parameters for binary Pitzer interaction parameters are not listed in this memo unless those parameters were specifically derived for inclusion in the database. The reference section provides the analysis reports and memos where complete listings of the parameters included in the QA database may be found, please refer to these references, or the data blocks listed in Appendix A, as a complete source of the parameter values included in DATA0.FM2.

AP-154 Tasks
The tasks completed under AP-154 and listed in AP-173 for inclusion in DATA0.FM2 are tabulated in Table 1.

Table 1. AP-154 Comparison of the documented parameters with those estimated using DATA0.FM2.

AP-154 Task	Chemical Entity	Fitting Parameter	Documented Value	Estimated with DATA0.FM2	Comments
14 & 15	Cerussite	Log K	-3.411	-3.312	Due to the greater than 10% difference for some of the Pitzer parameters it was decided that the Xiong(2014a) would be revised to reflect the values obtained using DATA0.FM2. The reason being the need to maintain consistency with the lead hydroxyl parameters derived under AP-155, Task 3 and 4.1.
	Na^+ - $Pb(CO_3)_2^{2-}$	$\beta^{(0)}$	0.6245	0.198	
		C^ϕ	-0.3633	-0.211	
	Na^+ - $Pb(CO_3)Cl^-$	$\beta^{(0)}$	0.0191	0.380	
		C^ϕ	0.229	0.192	
	HCO_3^- - $Pb(CO_3)_2^{2-}$	θ	0.108	0.148	
	CO_3^{2-} - $Pb(CO_3)_2^{2-}$	θ	0.0124	0.222	
18 & 19[1]	Na^+ - $PbEDTA^{2-}$	$\beta^{(0)}$	0.651	0.583	The difference in the parameters did not exceed 10%, therefore, the original documented parameters (Xiong 2014b) were retained in DATA0.FM2. Note that an error was found in the Mg^{2+} - $PbEDTA^{2-}$ parameter block that was corrected, and which did not affect the fitted parameters.
		C^ϕ	0.0647	0.0709	
	Mg^{2+} - $PbEDTA^{2-}$	$\beta^{(0)}$	1.840	2.422	
		C^ϕ	-0.150	-0.133	
20 & 21	Na^+ - $PbCit^-$	$\beta^{(0)}$	0.535	0.514	The difference in the parameters did not exceed 10%, therefore, the original parameters (Xiong 2014c) were retained in DATA0.FM2.
		C^ϕ	0.020	0.0248	
	Mg^{2+} - $PbCit^-$	$\beta^{(0)}$	1.975	1.903	
		C^ϕ	0.0771	0.0824	
22 & 24	See text below				
23	Mg^{2+} - $PbCl_3^-$	$\beta^{(0)}$	1.428	1.428	The values are identical, therefore, the original values (Xiong 2015) are retained in DATA0.FM2.
	MgOxalate(aq) - Mg^{2+}	λ	0.745	0.745	
	Cl^- - $PbCl_3^-$	θ	0.737	0.737	
	Mg^{2+} - $PbCl^+$ - Cl^-	Ψ	-0.413	-0.413	
30 & 31[1]	$Ca_2EDTA(s)$	Log K	-15.390	-15.390	The values are identical, therefore, the original values (Xiong 2015) were retained in DATA0.FM2. Note that an error was found in the Mg^{2+} / $CaEDTA^{2-}$ parameter block that was corrected, and which did not affect the fit.
	Mg^{2+} - $EDTA^{4-}$	$\beta^{(0)}$	-0.0100	-0.0100	
		C^ϕ	0.300	0.300	
	Mg^{2+} - $CaEDTA^{2-}$	$\beta^{(0)}$	0.525	0.525	
	Ca^{2+} - $MgEDTA^{2-}$	$\beta^{(0)}$	0.0844	0.0844	
	$CaEDTA^{2-}$	Log K	-11.156	-11.156	
	Na^+ - $CaEDTA^{2-}$	$\beta^{(0)}$	-0.00956	-0.00956	
		C^ϕ	0.0131	0.0131	
28 & 35[1]	Earlandite	Log K	-18.111	-18.106	An error was found in the Mg^{2+} - $Citrate^{3-}$ parameter block that required these parameters to be re-fit. The analysis report and accompanying memos were updated, and DATA0.FM2 was updated to reflect the new values. Note that AP-154 Tasks 20 and 21 were re-run with the updated database and there was no change in the parameters.
	Mg^{2+} - $MgCitrate^-$	$\beta^{(0)}$	0.865	1.0915	
	Mg^{2+} - $CaCitrate^-$	$\beta^{(0)}$	0.434	0.376	
	Mg^{2+} - $Citrate^{3-}$	$\beta^{(0)}$	3.241	0.933	
	$CaCitrate^-$	Log K	-4.973	-5.001	The difference in the parameters did not exceed 10%, therefore, the original values (Xiong 2012a) were retained in DATA0.FM2.
	Na^+ - $CaCitrate^-$	$\beta^{(0)}$	-0.131	-0.142	
		C^ϕ	-0.00682	-0.00346	
	Na^+ - Ca^{2+} - ClO_4^-	Ψ	0.157	0.144	

1 – During review it was found that the parameter blocks for Mg^{2+} - $PbEDTA^{2-}$, Mg^{2+} - $CaEDTA^{2-}$ and Mg^{2+} - $Citrate^{3-}$ had the alpha(1) set to 2.0 when it should have been 1.4, this was corrected, and had no impact on Tasks 18 and 19, and 30 and 31, however, it did effect Tasks 28 and 35 and new parameters were calculated and the accompanying documentation was updated.

AP-154 Tasks 22 and 24

Task 22 and 24 of AP154 are not included in Table 1 because the parameters were estimated by manual fitting (Xiong 2011a), and not by the use of the Python script, thus, it was not possible to run the Python script using DATA0.FM2 for parameter comparison purposes. Rather the test cases from Xiong 2011a were run in EQ3/6 using DATA0.FM2 and the output data were plotted together with the experimental data and predicted data of Xiong 2011a in Figure 1. Figure 1 shows that the predicted data of Xiong 2011a, and the predicted data using DATA0.FM2 are very close, therefore, the original parameter values of Xiong were retained in DATA0.FM2.

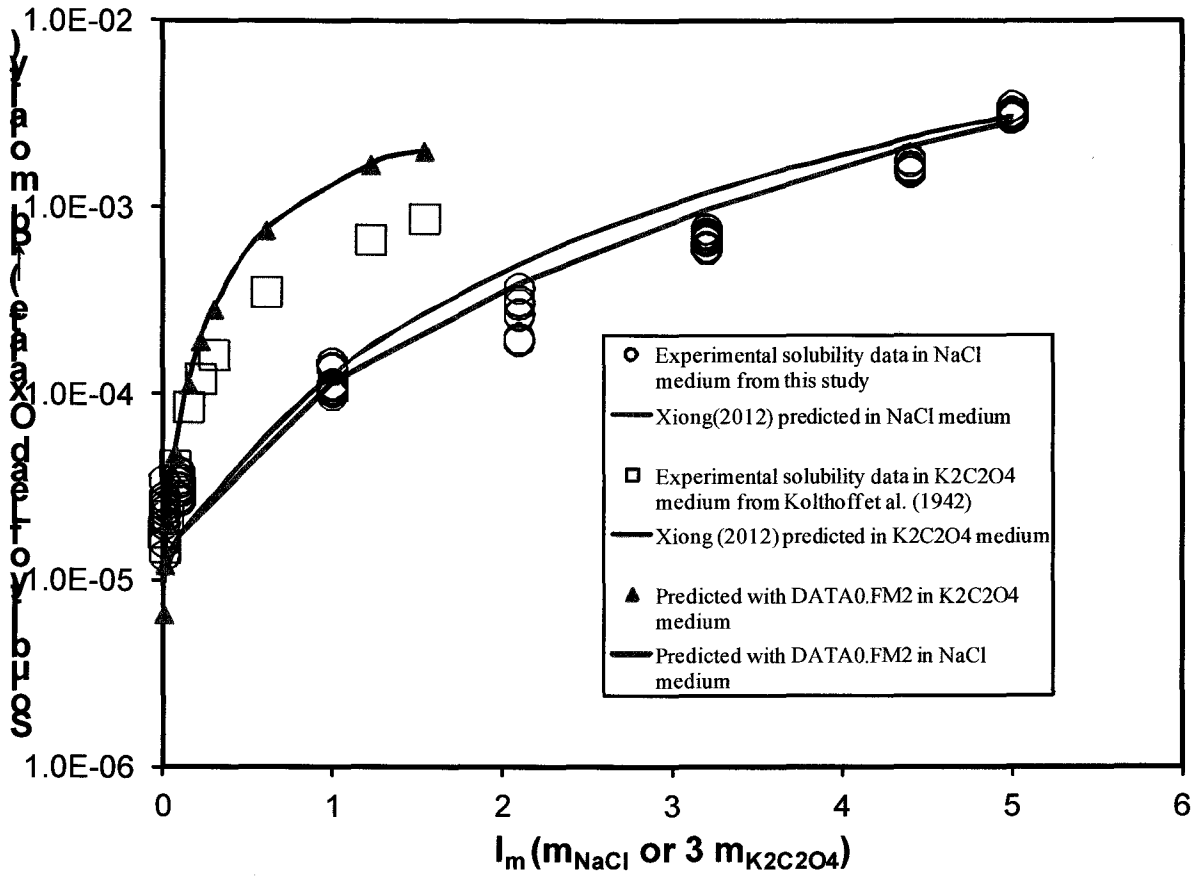

Figure 1. Comparison of the documented fit (Xiong, 2011a) with the DATA0.FM2 fit to the experimental data for AP-154 Task 22 and 24.

AP-154 Tasks 29 and 32

Note that tasks 29 and 32 from AP-154, which were specified by AP-173 to be included in DATA0.FM2 were not included because the parameters from these tasks were included in AP-154 tasks 30 and 31 for the EDTA parameters, and task 23 for the oxalate parameters, this is a deviation from AP-173.

AP-155 Tasks

The tasks completed under AP-155 and listed in AP-173 for inclusion in DATA0.FM2 are tabulated in Table 2.

Table 2. AP-155 Comparison of the documented parameters with those estimated using DATA0.FM2.

AP-155 Task	Chemical Entity	Fitting Parameter	Documented Value	Estimated with DATA0.FM2	Comments
3, 4.1	$Pb(OH)_2(aq)$	Log K	17.0475	17.0395	The difference in the parameters did not exceed 10%, therefore, the original values (Xiong 2015a) were retained in DATA0.FM2.
	$Pb(OH)_3^-$		27.989	27.992	
3, 4.1	$Na^+ - Pb(OH)_3^-$	$\beta^{(0)}$	0.335	0.335	The values are identical, therefore, the original values (Xiong 2015a) are retained in DATA0.FM2.
	$Pb(OH)_2(aq) - Cl^-$	λ	-0.172	-0.172	

AP-155 Task	Chemical Entity	Fitting Parameter	Documented Value	Estimated with DATA0.FM2	Comments
4.4, 4.11	$PbCl_2(aq) - Mg^{2+} - Cl^-$	ζ	0.682	0.682	The values are identical, therefore, the original values (Xiong 2015a) are retained in DATA0.FM2.
	$PbB_4O_7(aq) - Mg^{2+}$	λ	-0.365	-0.365	
4.2	$Pb(OH)_2(aq) - SO_4^{2-}$	λ	-0.558	-0.558	The values are identical, therefore, the original values (Xiong 2015a) are retained in DATA0.FM2.
	$Pb(OH)_3^- - SO_4^{2-}$	θ	-0.405	-0.405	
1	Pb_Metaborate_hydrate	Log K	-12.155	-12.16	The values are identical, therefore, the original values (Xiong 2015a) are retained in DATA0.FM2.
3,4.10 ,4.11	$PbB_4O_7(aq)$	Log K	-28.135	-28.149	The difference in the parameters did not exceed 10%, therefore, the original values (Xiong 2015a) were retained in DATA0.FM2.
4.10	$PbB_4O_7(aq) - Na+$	λ	0.156	0.0836	The value estimated with DATA0.FM2 is outside of the 10% range, however, the original documented value (Xiong 2015a) will be retained in DATA0.FM2 because it was derived in a step-wise manner and to change it would not be consistent with the original fitting scheme.
4.5	$MgSO_4(aq)$	Log K	-2.383	-2.389	The difference in the parameters did not exceed 10%, therefore, the original values (Xiong 2015a) were retained in DATA0.FM2.
	$MgB(OH)_4^+ - SO_4^{2-}$	$\beta^{(0)}$	0.781	0.825	
4.6	$Na^+ - Ca^{2+} - OH^-$	Ψ	-0.0198	-0.0198	The values are identical, therefore, the original values (Xiong 2015a) are retained in DATA0.FM2.
	$SO_4^{2-} - OH^- - Ca^{2+}$		0.0453	0.0453	
4.8	Na_Mg_Tetraborate(A)	Log K	-24.400	-24.420	The difference in the parameters did not exceed 10%, therefore, the original values (Xiong 2015a) were retained in DATA0.FM2.
4.8	Na_Mg_Tetraborate(B)	Log K	-24.990	-25.010	The difference in the parameters did not exceed 10%, therefore, the original values (Xiong 2015a) were retained in DATA0.FM2.
	$Mg^{2+} - B_3O_3(OH)_4^-$	$\beta^{(0)}$	0.987	0.987	
	$Mg^{2+} - B_3O_3(OH)_4^-$	C^{ϕ}	0.0100	0.0100	
4.9	$Na^+ - MgB(OH)_4^+$	θ	-0.298	-0.298	The values are identical, therefore, the original values (Xiong 2015a) are retained in DATA0.FM2.
	$B(OH)_3(aq) - Mg^{2+} - Cl^-$	ζ	0.00793	0.00793	
4.12	$B(OH)_3(aq) - B(OH)_3(aq) - PbCl_2(aq)$	μ	0.0350	0.0350	The values are identical, therefore, the original values (Xiong 2015a) are retained in DATA0.FM2.
4.7 (10)[1]	Na-Tetraborate	Log K	-24.800	-24.800	The difference in the parameters did not exceed 10%, therefore, the original values (Xiong 2012) were retained in DATA0.FM2.
	$NaB(OH)_4(aq) - Na^+$	λ	0.0930	0.0980	
	$SO_4^{-2} - B_4O_5(OH)_4^{-2} - Na^+$	Ψ	0.293	0.305	

1 – This task was completed under revision 0 of AP-155 which at the time had this task labeled as Task 10.

AP-173 Parameters

AP-173 specifies additional parameters to be included in DATA0.FM2, these parameters are listed in Table 3.

Table 3. Additional parameters to be included in DATA0.FM2.

Description	Reference
Hydromagnesite (5424) Log K_{sp}	Xiong 2015b
Pitzer binary interaction parameter Na^+ - $Am(EDTA)^-$	Xiong 2013a
Pitzer binary interaction parameter $AmHB_4O_7^{2+}$ - Cl^- $4B(OH)_4^- + 3H^+ + Am^{3+} = AmHB_4O_7^{2+} + 9H_2O(l)$	Domski and Xiong 2015, Xiong 2015c

Hydromagnesite(5424)

Xiong (2015b) derived the solubility product (log K_{sp}) for the Pitzer model according to the following dissolution expression:

(1) $Mg_5(CO_3)_4(OH)_2 \bullet 4H_2O + 10H^+ \rightleftharpoons 5Mg^{2+} + 4CO_2(g) + 10H_2O(l)$ $\log K_{sp} = 60.61$

However, to incorporate this value into the EQ3/6 database it was necessary to recast this expression in terms of the basis species for carbonate which is the bicarbonate ion (HCO_3^-). To convert to the basis species, HCO_3^-, the following reaction (2) was added to reaction (1), as follows:

(2) $4\ x(CO_2(g) + H_2O = H^+ + HCO_3^-$ $\log K = -7.8193)$

$4x(-7.8193) + 60.61 = 29.3328$

(3) $Mg_5(CO_3)_4(OH)_2 \bullet 4H_2O + 6H^+ \rightleftharpoons 5Mg^{2+} + 4HCO_3^- + 6H_2O(l)$ $\log K_{sp} = 29.3328$

Na^+ - $Am(EDTA)^-$ Pitzer binary interaction parameter

The following data block was added to DATA0.FM2 as calculated in Xiong (2013a).

```
+--------------------------------------------------------------------
Na+                          AmEDTA-
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0)
    a1 = 0.4372
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 0.29
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = -0.01303
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: "Calculations of Thermodynamic Parameters in EDTA System for Experimental
Data From
* Carlsbad Environmental Monitoring and Research Center (CEMRC)" ERMS:560761
+--------------------------------------------------------------------
```

$AmHB_4O_7^{2+}$ - Cl^- Pitzer binary interaction parameter

As required by AP-173, the binary Pitzer interaction parameters as documented in Xiong (2015) were included in the DATA0.FM2. The comparison of the documented parameter values (Xiong 2015) with those estimated using DATA0.FM2 is listed in Table 4.

Table 4. AP-173 Comparison of the documented parameters with those estimated using DATA0.FM2.

Chemical Entity	Parameter	Documented Value	Estimated with DATA0.FM2	Comments
$AmHB_4O_7^{2+}$	Log K	-37.34	-37.34	The values are identical, therefore, the original values (Xiong 2015c) are retained in DATA0.FM2.
$AmHB_4O_7^{2+}$ - Cl^-	$\beta^{(0)}$	0.92	0.92	

Files

The files that are to be submitted to the records center are listed in Table 5 and may be found at:
/nfs/data/CVSLIB/WIPP_EXTERNAL/ap173/Files

Table 5. List of files to be submitted to records.

File Name	Purpose
DATA0.FM2	QA database
FM2_additions.txt	Data blocks added to DATA0.FM1
Results_AP154_Task14-15_rev1.xlsx	Files which compare the documented parameters with those estimated using DATA0.FM2
Results_Task_18-19.xlsx	
Results_Task_20-21.xlsx	
AR_AP154_Task22_Modeling.xlsx	
AP154_Task23_Results.xlsx	
Results_AP154_Task30.xlsx	
Results_AP154_Task28-35.xlsx	
Results_AP155_task10_Na2B4O7_Na2SO4.xlsx	
Results_AP155_Task10_Na2B4O7_NaCl.xlsx	
Results_AP-155.xlsx	

References

Domski, P. S. and Y.-L. Xiong, 2015. "Analysis Plan for the Compilation and Testing of Selected Parameters from AP-134, Revision 3, AP-154, Revision 2 and AP-155, Revision 3 for Incorporation in a New QA EQ3/6 Thermodynamic Database" AP-154, Revision 1. Carlsbad, NM: Sandia National Laboratories. ERMS: 564585.

Kirchner, T.B., 2012. User's Manual for The EQ3CodeModule Version 1.00. Carlsbad, NM: Sandia National Laboratories. ERMS 557360.

Kolthoff, I.M., Perlich, R.W., and Weiblen, D., 1942. The solubility of lead sulfate and of lead oxalate in various media. Journal of Physical Chemistry **46**, 561–570.

Xiong, Y.-L. 2011. "Release of EQ3/6 Database DATA0.FM1." E-mail to Jennifer Long, March 9, 2011. Carlsbad, NM: Sandia National Laboratories. ERMS 555152.

Xiong, Y.-L. 2011a. "Experimental determination of solubilities of crystalline lead oxalate, PbC_2O_4(cr), in the NaCl–H2O system." Work Carried Out under Tasks 22 and 24 of AP-154: Analysis Plan for Derivation of Thermodynamic Properties Including Pitzer Parameters for Solubility Studies

of Iron, Lead and EDTA. To be included in the AP-154 records package. Carlsbad, NM: Sandia National Laboratories. SAND2011-9321J.

Xiong, Y.-L. 2012. "Thermodynamic Model for the Na–B(OH)3–Cl–SO4 system. Work Carried Out under Task 10 of the Analysis Plan for Thermodynamic Properties Including Pitzer Parameters for Solubility Studies of Borate." Carlsbad, NM: Sandia National Laboratories. ERMS: 558556.

Xiong, Y.-L., 2012a. "Experimental determination of solubility constant of di-calcium ethylenediaminetetraacentic acid (Ca2EDTA), Ca2C10H12N2O8(s), in the NaCl–H2O system. Work Carried Out under Task 29 of AP-154: Analysis Plan for Derivation of Thermodynamic Properties Including Pitzer Parameters for Solubility Studies of Iron, Lead and EDTA. To be included in the AP-154 records package". Carlsbad, NM: Sandia National Laboratories. ERMS: 558669.

Xiong, Y.-L. 2013. "Analysis Plan for Derivation of Thermodynamic Properties Including Pitzer Parameters for Solubility Studies of Iron, Lead, and EDTA" AP-154, Revision 2. Carlsbad, NM: Sandia National Laboratories. ERMS: 561114.

Xiong, Y.-L., 2013a. "Calculations of Thermodynamic Parameters in EDTA System for Experimental Data From Carlsbad Environmental Monitoring and Research Center (CEMRC)". Memo to WIPP Records Center. Carlsbad, NM: Sandia National Laboratories. ERMS 560761.

Xiong, Y.-L. 2014. "Analysis Plan for Derivation of Thermodynamic Properties Including Pitzer Parameters for Solubility Studies of Borate" AP-155, Revision 3. Carlsbad, NM: Sandia National Laboratories. ERMS: 562807

Xiong, Y.-L. 2014a. "Experimental and Thermodynamic Modeling Solubility of Cerussite, PbCO3(cr), in the Carbonate System to High Ionic Strengths." Carlsbad, NM: Sandia National Laboratories. ERMS: 561917

Xiong, Y.-L. 2014b. "Experimental and Thermodynamic Modeling of PbEDTA2– Interactions in NaCl and $MgCl_2$ Solutions." Carlsbad, NM: Sandia National Laboratories. ERMS: 562877

Xiong, Y.-L. 2014c. "Experimental and Thermodynamic Modeling of PbCit– Interactions in NaCl and MgCl2 Solutions" Carlsbad, NM: Sandia National Laboratories. ERMS: 562836

Xiong, Y.-L. 2015. "Experimental determination of solubilities of lead oxalate (PbC2O4), di-calcium ethylenediaminetetraacetic acid (Ca2EDTA(s)) in MgCl2–H2O system, and earlandite (Ca3[C3H5O(COO)3]2•4H2O) in NaCl–H2O and MgCl2–H2O systems, and their respective Pitzer interaction parameters. Revision 1, Supercedes ERMS 561917" Work Carried Out under Tasks 23, 28, 29, 30, 31 and 35 of AP-154: Analysis Plan for Derivation of Thermodynamic Properties Including Pitzer Parameters for Solubility Studies of Iron, Lead and EDTA. To be included in the AP-154 records packageAP-154, Revision 2. Carlsbad, NM: Sandia National Laboratories. ERMS: 564844.

Xiong, Y.-L. 2015a. "Derivation of Thermodynamic Parameters in Borate Systems for Experimental Data Under TP10-01. To be included in the AP-155 records package AP-154, Revision 2. Carlsbad, NM: Sandia National Laboratories. ERMS: 564800.

Xiong, Y.-L. 2015b. "Recalculation of Solubility Constants of Synthetic Hydromagnesite(5424) Using the Pitzer Model". Carlsbad, NM: Sandia National Laboratories. ERMS: 564356.

Xiong, Y.-L. 2015c. "Modeling Equilibrium Constant for $AmHB_4O_7^{2+}$ by Reevaluation of the Nd(III) Data for $NdHB_4O_7^{2+}$, and its Associated Pitzer Parameters to be Consistent with the WIPP Thermodynamic Model". Carlsbad, NM: Sandia National Laboratories. ERMS: 564857.

APPENDIX A.

Text and Data Blocks Added to DATA0.FM1

```
data0.fm2
Pitzer Thermodynamic Databse (10/14/2015)
DATA0.FM2 was created from DATA0.FM1 (DATA0.FMT.R2) to include all of the parameters
outlined in AP-173, revision 1.  This database was created in response to EPA comments
of the CRA-2014 and will be used to perform the PABC-2016 calculations.
+---------------------------------------------------------------------
AmHB4O7++                       Cl-
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0)
    a1 = 0.9163
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 1.74
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: AP-173
+---------------------------------------------------------------------
Na+                             PbCitrate-
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0)
    a1 = 0.535
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 0.29
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = 0.0196
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Fitting parameter for Tasks 20 & 21
+---------------------------------------------------------------------
Mg++                            PbCitrate-
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0)
    a1 = 1.97
    a2 = 0.
    a3 = 0.
    a4 = 0.
```

```
  beta(1)
    a1 = 1.74
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = 0.0771
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Fitting parameter for Tasks 20 & 21
+---------------------------------------------------------------------
Na+                           PbEDTA--
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0)
    a1 = 0.6507
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 1.74
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = 0.0647
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Fitting parameter for Tasks 18 & 19
+---------------------------------------------------------------------
Mg++                          PbEDTA--
  alpha(1) = 1.4
  alpha(2) = 12.0
  beta(0)
    a1 = 1.8399
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 3.27
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 =  -0.1501
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Fitting parameter for Tasks 18 & 19
+---------------------------------------------------------------------
Na+                           Pb(CO3)2--
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0)
    a1 = 0.1975
```

```
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 1.74
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = -0.2105
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Fitting parameter AP-154 Task 14 & 15
+----------------------------------------------------------------
Na+                          Pb(CO3)Cl-
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0)
    a1 = 0.3799
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 0.29
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = 0.1921
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Fitting parameter AP-154 Task 14 & 15
+----------------------------------------------------------------
Mg++                         B3O3(OH)4-
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0)
    a1 = 0.987
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 1.74
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = 0.01
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Xiong 2015 fitting solubility of Na2B4O7.10H2O data in
* MgCl2 solutions.  Based on average 1:2 and 2:1 interactions.
* beta(zero), a(1)=0.418; beta(one), a(1)=1.74.
+----------------------------------------------------------------
```

```
Mg++                          B4O5(OH)4--
  alpha(1) = 2.0
  alpha(2) = 7.59
  beta(0)
    a1 = -1.42258
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 14.3542
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 504.233
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = -0.62469
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Yin et al., 2007
+----------------------------------------------------------------------
MgB(OH)4+                     SO4--
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0)
    a1 = 0.7806
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 1.74
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Xiong (2015)
+----------------------------------------------------------------------
Mg++                          PbCl3-
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0)
    a1 = 1.4277
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 1.74
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = 0.000
    a2 = 0.
    a3 = 0.
```

```
    a4 = 0.
* Source: In Felmy et al. (2000), beta(zero), a(1) = 0.21.
+------------------------------------------------------------------
Na+                          Pb(Oxalate)2--
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0)
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = -1.86
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = 0.198
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: AP-154 Task 22 & 24
+------------------------------------------------------------------
K+                           Pb(Oxalate)2--
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0)
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = -1.86
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = 0.198
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: AP-154 Task 22 & 24
+------------------------------------------------------------------
Pb++                         Cl-
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0)
    a1 = 0.26
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 1.64
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
```

```
    a1 = 0.088
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: 84Millero/Byrne
+------------------------------------------------------------------
PbCl+                          Cl-
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0)
    a1 = 0.15
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: 84Millero/Byrne
+------------------------------------------------------------------
Na+                            PbCl3-
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0)
    a1 = -0.0605
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 0.00
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = 0.091
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: 84Millero/Byrne has a value of -0.19 for beta(0);
* Cphi evalauted by Xiong (2011)
+------------------------------------------------------------------
H+                             PbCl3-
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0)
    a1 = 0.27
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = -0.63
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.
```

```
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = 0.0000
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: 00Felmy et al.
+-----------------------------------------------------------------
Na+                          Pb(OH)3-
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0)
    a1 = 0.3354
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 0.29
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source:
*         Xiong (2015), modeling solubility of lead oxide in
*         NaClO4 and NaCl solutions in alkaline pH.
+-----------------------------------------------------------------
PbOH+                        Cl-
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0)
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = 0.0000
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Xiong (2015), modeling solubility of lead oxide in
*   NaCl solutions at high pH ranges.
+-----------------------------------------------------------------
Na+                          AmEDTA-
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0)
    a1 = 0.4372

    a2 = 0.
    a3 = 0.
    a4 = 0.
```

```
  beta(1)
    a1 = 0.29
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = -0.01303

    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: "Calculations of Thermodynamic Parameters in EDTA System for Experimental Data From
* Carlsbad Environmental Monitoring and Research Center (CEMRC)" ERMS:560761
+-----------------------------------------------------------------
Na+                          CaCitrate-
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0)
    a1 = -0.13133

    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 0.29
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = -0.006818
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Fitting parameter Task 35 AP-154
+-----------------------------------------------------------------
Mg++                         CaCitrate-
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0)
    a1 = 0.3760
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 1.74
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Fitting parameter Task 35 AP-154
+-----------------------------------------------------------------
Mg++                         MgCitrate-
  alpha(1) = 2.0
```

```
  alpha(2) = 12.0
  beta(0)
    a1 = 1.0915
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 1.74
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Xiong (2014) modeling solubility of earlandite in MgCl2
*   solutions.
+------------------------------------------------------------------
Mg++                          Citrate---
  alpha(1) = 1.4
  alpha(2) = 12.0
  beta(0)
    a1 = 0.9330
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 4.4
    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: Evaluated from earlanidite solubility in MgCl2.

+------------------------------------------------------------------
Na+                           CaEDTA--
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0)
    a1 = -0.00956
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 1.74
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = 0.01312
    a2 = 0.
```

```
    a3 = 0.
    a4 = 0.
* Source: AP-154 Task 30.
+-------------------------------------------------------------------
Mg++                          CaEDTA--
  alpha(1) = 1.4
  alpha(2) = 12.0
  beta(0)
    a1 = 0.525
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 3.27
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: AP-154 Task 30.
+-------------------------------------------------------------------
Ca++                          MgEDTA--
  alpha(1) = 1.4
  alpha(2) = 12.0
  beta(0)
    a1 = 0.0844
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 3.27
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Xiong (2014)
+-------------------------------------------------------------------
Mg++                          EDTA----
  alpha(1) = 1.4
  alpha(2) = 12.0
  beta(0)
    a1 = -0.01
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 11.6
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
```

```
  Cphi:
    a1 = 0.30

    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Xiong (2015) AP-154 Task 28 & 35

+-----------------------------------------------------------------
Na+                         MgB(OH)4+
  theta:
    a1 = -0.2975
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Xiong (2015), modeling solubility of "Na-Mg-Tetraborate
*   (B)" in MgCl2 solutions
+-----------------------------------------------------------------
Mg++                        PbCl+
  theta:
    a1 = -0.13
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: 00Felmy, -0.13.
+-----------------------------------------------------------------
Na+                         Pb++
  theta:
    a1 = 0.10
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: 84Millero/Byrne set to 0; 00Felmy has a value of 0.10
+-----------------------------------------------------------------
Na+                         PbCl+
  theta:
    a1 = 0.000
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: 84Millero/Byrne
+-----------------------------------------------------------------
HCO3-                       Pb(CO3)2--
  theta:
    a1 = 0.1476
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Fitting parameter AP-154 Task 14 & 15
+-----------------------------------------------------------------
Cl-                         PbCl3-
  theta:
    a1 = 0.7371
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Xiong (2014), modeling lead oxalate solubility in
*   MgCl2 solutions.
+-----------------------------------------------------------------
SO4--                       B(OH)4-
  theta:
    a1 = 0.1697
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Evaluated from sodium tetraborate in Na2SO4 solutions.
* In FW86, the value is -0.012. The value for the revised model
* is 0.1697.
+-----------------------------------------------------------------
SO4--                       Pb(OH)3-
  theta:
    a1 = -0.4046
```

```
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Xiong (2015), modeling solubility of lead oxide in
*         Na2SO4 solutions.
+------------------------------------------------------------------
CO3--                       Pb(CO3)2--
  theta:
    a1 = 0.2223
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Fitting parameter AP-154 Task 14 & 15
+------------------------------------------------------------------
PbOxalate(aq)               Na+
  lambda:
    a1 = 0.00
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Setting to zero
+------------------------------------------------------------------
PbCO3(aq)                   Na+
  lambda:
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Woosley and Millero (2013)
+------------------------------------------------------------------
B(OH)3(aq)                  Mg++
  lambda:
    a1 =  0.0000E+00
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Xiong 2015 fitting solubility of Na2B4O7.10H2O in
* MgCl2 solutions
+------------------------------------------------------------------
MgOxalate(aq)               Mg++
  lambda:
    a1 = 0.7454
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source:
+------------------------------------------------------------------
NaB(OH)4(aq)                Na+
  lambda:
    a1 = 0.093
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Task 10, AP-155 fit value = 0.093
+------------------------------------------------------------------
PbB4O7(aq)                  Mg++
  lambda:
    a1 = -0.3653
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Xiong (2015), modeling solubility of lead solubility in
*         MgCl2 solutions with 0.3 m H3BO3.
*
*
+------------------------------------------------------------------
MgSO4(aq)                   Mg++
  lambda:
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
```

```
* Source: Xiong (2015) modeling solubility of brucite in Na2SO4
*   solutions in presence of boric acid
+--------------------------------------------------------------
PbB4O7(aq)                  Na+
  lambda:
    a1 = 0.1555
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Xiong (2015) AP-155
+--------------------------------------------------------------
B(OH)3(aq)                  Pb++
  lambda:
    a1 = 0.2925
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Xiong (2015) modeling lead solubility in boric acid,
*         Set to 0.2925 in analog to H4SiO4/Mg++ from 97Aza/Fou.
+--------------------------------------------------------------
B(OH)3(aq)                  PbB(OH)4+
  lambda:
    a1 = 0.0925
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Xiong (2015) modeling lead solubility in boric acid.
*         Set to 0.0925 in analog to H4SiO4/Mg++ from 97Aza/Fou
+--------------------------------------------------------------
PbCl2(aq)                   Mg++
  lambda:
    a1 = -0.071
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: 00Felmy, -0.071. Xiong (2015) modeling
+--------------------------------------------------------------
PbCl2(aq)                   Na+
  lambda:
    a1 = -0.11
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: 84Millero/Byrne has a value of -0.14;
* 00Felmy has a value of -0.11
+--------------------------------------------------------------
Pb(OH)2(aq)                 Na+
  lambda:
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source:
*         Xiong (2015), modeling solubility of lead oxide in
*         NaCl and NaClO4 solutions.
+--------------------------------------------------------------
PbCO3(aq)                   Cl-
  lambda:
    a1 = -0.020
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Woosley and Millero (2013)
+--------------------------------------------------------------
PbOxalate(aq)               Cl-
  lambda:
    a1 = 0.00000
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Setting to 0
+--------------------------------------------------------------
```

```
PbOxalate(aq)              Oxalate--
  lambda:
    a1 = 0.00000
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Setting to 0
+----------------------------------------------------------------
Pb(OH)2(aq)                SO4--
  lambda:
    a1 = -0.5581
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Xiong (2015), modeling solubility of lead oxide in
*         Na2SO4 solutions.
+----------------------------------------------------------------
Pb(OH)2(aq)                Cl-
  lambda:
    a1 = -0.1721
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Xiong (2015), modeling solubility of lead oxide in
*         NaCl and NaClO4 solutions.
+----------------------------------------------------------------
PbCl2(aq)                  Cl-
  lambda:
    a1 = -0.14
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Xiong 2011; Both 84Millero/Byrne and 00Felmy
* has a value of -0.11
+----------------------------------------------------------------
PbCl2(aq)

  lambda:
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
  mu:
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: [template only]
+----------------------------------------------------------------
PbCl2(aq)                  B(OH)3(aq)
  lambda:
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Xiong (2015) modeling lead solubility in NaCl and
*         MgCl2 solutions with boric acid
+----------------------------------------------------------------
Na+                        Ca++                       ClO4-
  psi:
    a1 = 0.1574
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Fitting parameter Task 28&35c
+----------------------------------------------------------------
Na+                        Ca++                       OH-
  psi:
    a1 = -0.0198
    a2 = 0.
    a3 = 0.
    a4 = 0.
```

```
* Source: Xiong (2015) modeling solubility of portlandite in
*         Na2SO4 solutions with 0.001 m H3BO3.
+------------------------------------------------------------------
Mg++                        PbCl+                       Cl-
  psi:
    a1 = -0.4129
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Xiong (2015) Evaluated from lead solubility data
*         in MgCl2
+------------------------------------------------------------------
SO4--                       B4O5(OH)4--                 Na+
  psi:
    a1 = 0.293
    a2 = 0.
    a3 = 0.
    a4 = 0.
* a1 set to 0.00 for fitting
* Set to 0 for FW86 model.
+------------------------------------------------------------------
SO4--                       OH-                         Ca++
  psi:
    a1 = 0.04525
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Xiong (2015) modeling solubility of portlandite in
*   Na2SO4 solutions with boric acid.
+------------------------------------------------------------------
Cl-                         PbCl3-                      Mg++
  psi:
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Xiong (2015)
+------------------------------------------------------------------
PbCl2(aq)                   Na+                         Cl-
  zeta:
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Setting to zero
+------------------------------------------------------------------
PbOxalate(aq)               Na+                         Cl-
  zeta:
    a1 = 0.
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Setting to zero
+------------------------------------------------------------------
PbCO3(aq)                   Na+                         Cl-
  zeta:
    a1 = -0.145
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Woosley anf Millero (2013)
+------------------------------------------------------------------
B(OH)3(aq)                  Mg++                        Cl-
  zeta:
    a1 = 0.00793
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Xiong (2015) modeling sodium tetraborate in MgCl2+NaCl
*         solutions.
+------------------------------------------------------------------
PbCl2(aq)                   Mg++                        Cl-
```

```
  zeta:
    a1 = 0.6820
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Xiong (2015) modeling
*         -0.02340
+---------------------------------------------------------------
B(OH)3(aq)                B(OH)3(aq)                PbCl2(aq)
  mu:
    a1 = 0.035
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Xiong (2015) modeling lead metaborate hydrate solubility
*         in MgCl2+NaCl mixtures with 0.3 m H3BO3.
+---------------------------------------------------------------
Pb       207.20000
+---------------------------------------------------------------------
Pb++
     charge  =   2.0
****
     1 element(s):
      1.0000 Pb
****
+---------------------------------------------------------------------
AmHB4O7++                 AmHB4O7++
     charge  =   2.0
****
     4 element(s):
      1.0000 Am              1.0000 H              4.0000 B
      7.0000 O
****
     5 species in aqueous dissociation reaction:
    -1.0000  AmHB4O7++               -9.0000  H2O
     1.0000  Am+++                    3.0000  H+
     4.0000  B(OH)4-
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data  -37.3416   No_Data   No_Data
        No_Data   No_Data   No_Data   No_Data
* Source: AP-173
+---------------------------------------------------------------
PbEDTA--                  PbC10H12O8N2--
     charge  =  -2.0
****
     5 element(s):
     10.0000 C              1.0000 Pb            12.0000 H
      2.0000 N              8.0000 O
****
     3 species in aqueous dissociation reaction:
    -1.0000  PbEDTA--                 1.0000  Pb++
     1.0000  EDTA----
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data   20.0100   No_Data   No_Data
        No_Data   No_Data   No_Data   No_Data
* Source:
+---------------------------------------------------------------
PbCitrate-                PbC6H5O7-
     charge  =  -1.0
****
     4 element(s):
      6.0000 C              1.0000 Pb             5.0000 H
      7.0000 O
****
     3 species in aqueous dissociation reaction:
    -1.0000  PbCitrate-               1.0000  Pb++
     1.0000  Citrate---
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data   7.28      No_Data   No_Data
```

```
        No_Data    No_Data    No_Data    No_Data
* Source: Fit based on the values extrapolated to infinite dilution using the SIT model Task
20 & 21 AP-154
+---------------------------------------------------------------
PbCO3(aq)                    PbCO3(aq)
     charge   =    0.0
****
     3 element(s):
      1.0000 Pb              1.0000 C               3.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000   PbCO3(aq)                -1.0000   H+
     1.0000   Pb++                     1.0000   HCO3-
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data     3.4692    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Woosley and Millero (2013) have a
* value of 6.87 for log beta1, resulting in a value of 3.4692.
+---------------------------------------------------------------
Pb(CO3)2--                   Pb(CO3)2--
     charge   =   -2.0
****
     3 element(s):
      1.0000 Pb              2.0000 C               6.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000   Pb(CO3)2--               -2.0000   H+
     1.0000   Pb++                     2.0000   HCO3-
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data    10.2684    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Easley and Byrne (2011) obtained a value of 10.41 for
* the formation
* reaction, which leads to a value of 10.2684 in the above entry.
+---------------------------------------------------------------
Pb(CO3)Cl-                   Pb(CO3)Cl-
     charge   =   -1.0
****
     4 element(s):
      1.0000 Pb              1.0000 C               3.0000 O
      1.0000 Cl
****
     5 species in aqueous dissociation reaction:
    -1.0000   Pb(CO3)Cl-               -1.0000   H+
     1.0000   Pb++                     1.0000   HCO3-
     1.0000   Cl-
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data     3.1092    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source:
* Woosley and Millero (2013) has a value of 7.23+/-0.74 for CO3--,
* corresponding to -3.1092 in the entry.
+---------------------------------------------------------------
PbOxalate(aq)                PbC2O4(aq)
     charge   =    0.0
****
     3 element(s):
      2.0000 C               1.0000 Pb              4.0000 O
****
     3 species in aqueous dissociation reaction:
    -1.0000   PbOxalate(aq)             1.0000   Pb++
     1.0000   Oxalate--
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data    -5.8500    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Based on experments in NaCl solution
+---------------------------------------------------------------
Pb(Oxalate)2--               Pb(C2O4)2--
```

```
     charge   =   -2.0
****
     3 element(s):
      4.0000 C              1.0000 Pb             8.0000 O
****
     3 species in aqueous dissociation reaction:
    -1.0000   Pb(Oxalate)2--            1.0000   Pb++
     2.0000   Oxalate--
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data    -8.0500    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Based on experments in K2C2O4 solutions
+---------------------------------------------------------------------
NaB(OH)4(aq)                NaB(OH)4(aq)
     charge   =    0.0
****
     4 element(s):
      1.0000 B              4.0000 H              1.0000 Na
      4.0000 O
****
     3 species in aqueous dissociation reaction:
    -1.0000   NaB(OH)4(aq)                  1.0000   Na+
     1.0000   B(OH)4-
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data    -0.2500    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Xiong, 2012, SIT model to extrapolate Reardon (1976)
* conditional formation constants. logK = -0.25.  Set to No_Data
* for Felmy and Weare (1986) model.
+---------------------------------------------------------------------
MgSO4(aq)                   MgSO4(aq)
     charge   =    0.0
****
     3 element(s):
      1.0000 S              1.0000 Mg             4.0000 O
****
     3 species in aqueous dissociation reaction:
    -1.0000   MgSO4(aq)                 1.0000   Mg++
     1.0000   SO4--
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data    -2.3826    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Xiong (2005), modeling solubility of brucite in Na2SO4
*         solutions with 0.001 H3BO3. From Kratsis et al. (2001),
*         -2.38.
+---------------------------------------------------------------------
PbB4O7(aq)                  PbB4O7(aq)
     charge   =    0.0
****
     3 element(s):
      4.0000 B              1.0000 Pb             7.0000 O
****
     5 species in aqueous dissociation reaction:
    -1.0000   PbB4O7(aq)                  1.0000   Pb++
    -9.0000   H2O                         2.0000   H+
     4.0000   B(OH)4-
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data  -28.1354    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source:  Xiong (2015)
+---------------------------------------------------------------------
Pb(B(OH)4)3-                Pb(B(OH)4)3-
     charge   =   -1.0
****
     4 element(s):
      1.0000 Pb            12.0000 H             12.0000 O
      3.0000 B
****
```

```
     3 species in aqueous dissociation reaction:
    -1.0000  Pb(B(OH)4)3-              1.0000  Pb++
     3.0000  B(OH)4-
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data    99.9999    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Xiong (2015) modeling solubility of PbO
*         in the presence of boric acid.
*         Simultaneous fitting three data sets (two from Shchigol
*         and one from my work).
+---------------------------------------------------------------
PbB(OH)4+                  PbB(OH)4+
     charge  =   1.0
****
     4 element(s):
      1.0000 Pb             4.0000 H              4.0000 O
      1.0000 B
****
     3 species in aqueous dissociation reaction:
    -1.0000  PbB(OH)4+                 1.0000  Pb++
     1.0000  B(OH)4-
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data    -2.9500    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Xiong (2015) modeling solubility of PbO in NaCl
*         solutions in the presence of boric acid.
*         Using B dot equation to extrapolate the literature
*         value.
+---------------------------------------------------------------
Pb(B(OH)4)2(aq)            Pb(B(OH)4)2(aq)
     charge  =   0.0
****
     4 element(s):
      1.0000 Pb             8.0000 H              8.0000 O
      2.0000 B
****
     3 species in aqueous dissociation reaction:
    -1.0000  Pb(B(OH)4)2(aq)           1.0000  Pb++
     2.0000  B(OH)4-
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data    -5.5100    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Xiong (2015) modeling solubility of PbO in NaCl
*         solutions in the presence of boric acid.
*         Using B dot equation to extrapolate the literature
*         value.
+---------------------------------------------------------------
PbCl+                      PbCl+
     charge  =   1.0
****
     2 element(s):
      1.0000 Pb             1.0000 Cl
****
     3 species in aqueous dissociation reaction:
    -1.0000  PbCl+                     1.0000  Pb++
     1.0000  Cl-
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data    -1.4800    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: 07Luo/Millero
+---------------------------------------------------------------
PbCl2(aq)                  PbCl2(aq)
     charge  =   0.0
****
     2 element(s):
      1.0000 Pb             2.0000 Cl
****
     3 species in aqueous dissociation reaction:
```

```
    -1.0000  PbCl2(aq)                  1.0000  Pb++
     2.0000  Cl-
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data    -2.0300    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: 84Millero/Byrne
+---------------------------------------------------------------
PbCl3-                      PbCl3-
     charge  =   -1.0
****
     2 element(s):
      1.0000 Pb             3.0000 Cl
****
     3 species in aqueous dissociation reaction:
    -1.0000  PbCl3-                     1.0000  Pb++
     3.0000  Cl-
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data    -1.8600    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: 07Luo/Millero
+---------------------------------------------------------------
PbOH+                       PbOH+
     charge  =   1.0
****
     3 element(s):
      1.0000 Pb             1.0000 H              1.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  PbOH+                      -1.0000  H+
     1.0000  Pb++                        1.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data     7.4600    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Powell et al. (2009)
+---------------------------------------------------------------
Pb(OH)2(aq)                 Pb(OH)2(aq)
     charge  =   0.0
****
     3 element(s):
      1.0000 Pb             2.0000 H              2.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  Pb(OH)2(aq)                -2.0000  H+
     1.0000  Pb++                        2.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data    17.0475    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Powell et al. (2009), 16.94.
*         Xiong (2015), 17.0409
+---------------------------------------------------------------
Pb(OH)3-                    Pb(OH)3-
     charge  =  -1.0
****
     3 element(s):
      1.0000 Pb             3.0000 H              3.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  Pb(OH)3-                   -3.0000  H+
     1.0000  Pb++                        3.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data    27.9886    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: Powell et al. (2009), 28.03.  Xiong (2015), 28.0210
+---------------------------------------------------------------
AmEDTA-                     AmC10H12O8N2-
     charge  =  -1.0
****
```

```
     5 element(s):
      1.0000 Am            10.0000 C             12.0000 H
      2.0000 N              8.0000 O
****
     3 species in aqueous dissociation reaction:
    -1.0000  AmEDTA-                  1.0000  Am+++
     1.0000  EDTA----
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data  -20.5500   No_Data   No_Data
        No_Data   No_Data   No_Data   No_Data
* Source: Calculations of Thermodynamic Parameters in EDTA System for Experimental Data From
* Carlsbad Environmental Monitoring and Research Center (CEMRC). ERMS:560761
+---------------------------------------------------------------
CaCitrate-                CaC6H5O7-
     charge  =  -1.0
****
     4 element(s):
      6.0000 C              1.0000 Ca             5.0000 H
      7.0000 O
****
     3 species in aqueous dissociation reaction:
    -1.0000  CaCitrate-               1.0000  Ca++
     1.0000  Citrate---
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data   -4.9725   No_Data   No_Data
        No_Data   No_Data   No_Data   No_Data
* Source: AP-154 Task 35
+---------------------------------------------------------------
CaEDTA--                  CaC10H12O8N2--
     charge  =  -2.0
****
     5 element(s):
     10.0000 C              1.0000 Ca            12.0000 H
      2.0000 N              8.0000 O
****
     3 species in aqueous dissociation reaction:
    -1.0000  CaEDTA--                 1.0000  Ca++
     1.0000  EDTA----
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data  -11.1562   No_Data   No_Data
        No_Data   No_Data   No_Data   No_Data
* Source: AP-154 Task 30
+---------------------------------------------------------------
Cerussite(cr)                PbCO3(cr)
     sp.type =  solid
*    EQ3/6   =  pis
     revised =  16-jan-2013
*    mol.wt. =   570.134 g/mol
     V0PrTr  =   203.620 cm**3/mol [source:    ]
****
     3 element(s):
      1.0000 Pb             1.0000 C              3.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  Cerussite(cr)              -1.0000  H+
     1.0000  HCO3-                       1.0000  Pb++
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        500.0000  -3.3116   500.0000  500.0000
        500.0000  500.0000  500.0000  500.0000
*
*    Source: Xiong (2013) fitting
+---------------------------------------------------------------
Earlandite             Ca3Citrate2:4H2O
     sp.type =  solid
*    EQ3/6   =  hmo
     revised =  16-oct-2006
*    mol.wt. =   570.5008 g/mol
     V0PrTr  =     0.000 cm**3/mol [source:          ]
```

```
****
     4 element(s):
     12.0000 C             18.0000 H             18.0000 O
      3.0000 Ca
****
     4 species in aqueous dissociation reaction:
    -1.0000  Earlandite                  3.0000  Ca++
     2.0000  Citrate---                  4.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        500.0000  -18.1110  500.0000  500.0000
        500.0000  500.0000  500.0000  500.0000
+---------------------------------------------------------------
Ca2EDTA(s)                Ca2C10H12O8N2
     sp.type =  solid
*    EQ3/6   =  hmo
     revised =  26-Sept-2012
*    mol.wt. =   570.5008 g/mol
     V0PrTr  =     0.000 cm**3/mol [source:          ]
****
     5 element(s):
     10.0000 C             12.0000 H              8.0000 O
      2.0000 Ca             2.0000 N
****
     3 species in aqueous dissociation reaction:
    -1.0000  Ca2EDTA(s)                  2.0000  Ca++
     1.0000  EDTA----
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        500.0000  -15.3900  500.0000  500.0000
        500.0000  500.0000  500.0000  500.0000
+---------------------------------------------------------------
PbOxalate(cr)             PbC2O4
     V0PrTr  =   000.000 cm**3/mol [source:          ]
****
     3 element(s):
      2.0000 C              1.0000 Pb             4.0000 O
****
     3 species in aqueous dissociation reaction:
    -1.0000  PbOxalate(cr)               1.0000  Pb++
     1.0000  Oxalate--
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data  -11.1300   No_Data   No_Data
        No_Data   No_Data   No_Data   No_Data
* Source: Xiong (2011), evaluated from PbOxalate(cr) solubility in
* NaCl solutions.
+---------------------------------------------------------------
Na_Tetraborate            Na2B4O7.10H2O
     V0PrTr  =   000.000 cm**3/mol [source:          ]
****
     4 element(s):
      4.0000 B             20.0000 H              2.0000 Na
     17.0000 O
****
     5 species in aqueous dissociation reaction:
    -1.0000  Na_Tetraborate              1.0000  H2O
     2.0000  Na+                         4.0000  B(OH)4-
     2.0000  H+
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data   -24.800   No_Data   No_Data
        No_Data   No_Data   No_Data   No_Data
* Source: Log K set to 0.00 for fitting
*         In Felmy and Weare (1986) model, the value for borax is -24.4918.
+---------------------------------------------------------------
Na_Mg_Tetraborate(A)      Na1.8Mg0.1B4O7.10H2O
     V0PrTr  =   000.000 cm**3/mol [source:          ]
****
     5 element(s):
      4.0000 B             20.0000 H              1.8000 Na
     17.0000 O              0.1000 Mg
```

```
****
     6 species in aqueous dissociation reaction:
    -1.0000  Na_Mg_Tetraborate(A)       1.0000  H2O
     1.8000  Na+                        4.0000  B(OH)4-
     2.0000  H+                         0.1000  Mg++
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data  -24.4000   No_Data   No_Data
        No_Data   No_Data   No_Data   No_Data
* Source: Xiong (2015) Evaluated from solubility of Na2B4O7:10H2O
*         in MgCl2 solutions (log K = -24.4500).
*
*
*
+---------------------------------------------------------------------
Na_Mg_Tetraborate(B)      Na1.6Mg0.2B4O7.10H2O
     V0PrTr   =   000.000 cm**3/mol [source:         ]
****
     5 element(s):
      4.0000 B             20.0000 H             1.6000 Na
     17.0000 O              0.2000 Mg
****
     6 species in aqueous dissociation reaction:
    -1.0000  Na_Mg_Tetraborate(B)       1.0000  H2O
     1.6000  Na+                        4.0000  B(OH)4-
     2.0000  H+                         0.2000  Mg++
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
       -25.7250  -24.9900   No_Data   No_Data
        No_Data   No_Data   No_Data   No_Data
* Source: Xiong (2015) Evaluated from solubility of Na2B4O7:10H2O
*         in MgCl2 solutions (log K = -24.8000).
*
*
*
+---------------------------------------------------------------------
PbMgCl4:6H2O              PbMgCl4:6H2O
     V0PrTr   =   000.000 cm**3/mol [source:         ]
****
     5 element(s):
      4.0000 Cl             1.0000 Pb             1.0000 Mg
     12.0000 H              6.0000 O
****
     5 species in aqueous dissociation reaction:
    -1.0000  PbMgCl4:6H2O               1.0000  Pb++
     4.0000  Cl-                        1.0000  Mg++
     6.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data   99.9999   No_Data   No_Data
        No_Data   No_Data   No_Data   No_Data
* Source: Felmy et al., 2000, GCA, 64:3615-3628
*        No_Data   -6.0700   No_Data   No_Data
+---------------------------------------------------------------------
Pb_Metaborate_hydrate         Pb(BO2)2:H2O
     sp.type =  solid
*    EQ3/6   =  pis
     revised =  01-Jul-2015
*    mol.wt. =   xxxx g/mol
     V0PrTr  =   0.0 cm**3/mol [source:]
****
     4 element(s):
      1.0000 Pb             2.0000 B              5.0000 O
      2.0000 H
****
     4 species in aqueous dissociation reaction:
    -1.0000  Pb_Metaborate_hydrate       -3.0000  H2O
     2.0000  B(OH)4-                                          1.0000  Pb++
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data  -12.1551   No_Data   No_Data
        No_Data   No_Data   No_Data   No_Data
```

```
*Source: Xiong (2015)
+--------------------------------------------------------------------
Litharge                PbO
     sp.type =  solid   polymorph
*    EQ3/6   =  ymp.R2, ymp.R0, com, ree, alt, sup
     YMP Qualification status = Q
*    mol.wt. =   223.199 g/mol
     V0PrTr  =    23.910 cm**3/mol [source: 78hel/del]
****
     2 element(s):
      1.0000 O              1.0000 Pb
****
     4 species in aqueous dissociation reaction:
    -1.0000  Litharge                   -2.0000  H+
     1.0000  H2O                         1.0000  Pb++
*
**** logK grid [0-25-60-100C @1bar; 150-200-250-300C @Psat-H2O]:
        13.6341   12.5914   11.3804   10.2699
         9.1675    8.2762    7.5166    6.8252
+--------------------------------------------------------------------
Hydromagnesite5424        Mg5(CO3)4(OH)2.4H2O
     V0PrTr  =   000.000 cm**3/mol [source:         ]
****
     4 element(s):
      4.0000 C             10.0000 H             5.0000 Mg
     18.0000 O
****
     5 species in aqueous dissociation reaction:
    -1.0000  Hydromagnesite5424       -6.0000  H+
     5.0000  Mg++                      4.0000  HCO3-
     6.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data   29.3328   No_Data   No_Data
        No_Data   No_Data   No_Data   No_Data
* Source: Recalculation of Solubility Constants of Synthetic Hydromagnesite(5424) Using the
Pitzer Model
* Note that the reaction in the source was in terms of CO2(g) a non-basis species, to covert
to the basis species, HCO3-
* the reaction 4 x(CO2(g) + H2O = H+ + HCO3- logK = -7.8193) was added, 60.61 + 4 x -7.8193 =
29.3328

+--------------------------------------------------------------------
```

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to: SNL WIPP Records Center
Defense Waste Management Programs

from: Paul S. Domski

subject: Memo of Correction for *"Memo AP-173, EQ3/6 Database Update: DATA0.FM2"*

The purpose of this memo is document that "Memo AP-173, EQ3/6 Database Update: DATA0.FM2", file name "AP173_FM2_memo_final.doc", dated 10/27/2015 has been updated to correct a formatting error in Figure 1 where the Y-axis label would not print properly. The new file, "AP173_FM2_memo_final_fixed_fig.doc" differs from the original only in the way that Figure 1 prints.

AP-154 Tasks 22 and 24

Task 22 and 24 of AP154 are not included in Table 1 because the parameters were estimated by manual fitting (Xiong 2011a), and not by the use of the Python script, thus, it was not possible to run the Python script using DATA0.FM2 for parameter comparison purposes. Rather the test cases from Xiong 2011a were run in EQ3/6 using DATA0.FM2 and the output data were plotted together with the experimental data and predicted data of Xiong 2011a in Figure 1. Figure 1 shows that the predicted data of Xiong 2011a, and the predicted data using DATA0.FM2 are very close, therefore, the original parameter values of Xiong were retained in DATA0.FM2.

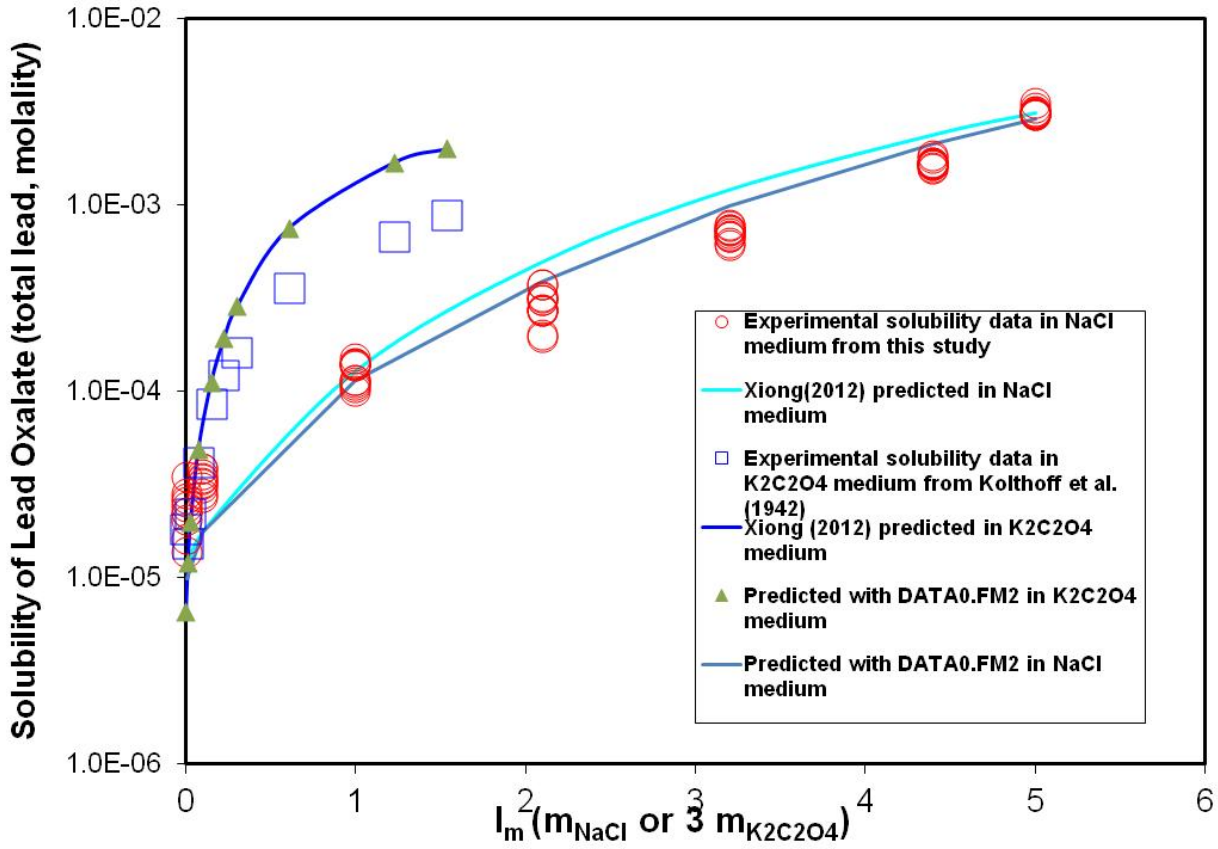

Figure 1. Comparison of the documented fit (Xiong, 2011a) with the DATA0.FM2 fit to the experimental data for AP-154 Task 22 and 24.

AP-154 Tasks 29 and 32

Note that tasks 29 and 32 from AP-154, which were specified by AP-173 to be included in DATA0.FM2 were not included because the parameters from these tasks were included in AP-154 tasks 30 and 31 for the EDTA parameters, and task 23 for the oxalate parameters, this is a deviation from AP-173.

AP-155 Tasks

The tasks completed under AP-155 and listed in AP-173 for inclusion in DATA0.FM2 are tabulated in Table 2.

Table 2. AP-155 Comparison of the documented parameters with those estimated using DATA0.FM2.

AP-155 Task	Chemical Entity	Fitting Parameter	Documented Value	Estimated with DATA0.FM2	Comments
3, 4.1	$Pb(OH)_2(aq)$	Log K	17.0475	17.0395	The difference in the parameters did not exceed 10%, therefore, the original values (Xiong 2015a) were retained in DATA0.FM2.
	$Pb(OH)_3^-$		27.989	27.992	
3, 4.1	$Na^+ - Pb(OH)_3^-$	$\beta^{(0)}$	0.335	0.335	The values are identical, therefore, the