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SANDIA NATIONAL LABORATORIES  
WASTE ISOLATION PILOT PLANT  

AP-154  
Revision 2  

Analysis Plan for Derivation of Thermodynamic Properties Including Pitzer Parameters for Solubility Studies of Iron, Lead and EDTA  

Task 4.4.2.2.1  

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1 Introduction and Objectives

1.1 Introduction

To model the solution chemistry for brines relevant to the WIPP repository, WIPP PA uses the Pitzer model (Pitzer 1973, 1975) to evaluate the activity coefficients for the various components of the brine. To date, the WIPP thermodynamic database does not incorporate iron, lead species, or sulfide species. There will be significant amounts of iron and lead present in the repository as a result of the steel used in the waste containers and lead used in shielded containers in the repository. In addition, sulfide, which could be produced by sulfate reduction, is expected to interact strongly with both lead and iron(II) by forming sulfide phases. Lead and iron(II) are expected to compete with the transuranic species in complexation of the organic ligands such as citrate, EDTA and oxalate. Consequently, it is desirable to model the WIPP brines to interaction with iron(II), lead and sulfide species. As a result, in order to predict accurately the chemical conditions in the repository, we must obtain the parameters necessary for such a modeling and incorporate the chemistry of iron, lead and sulfide into the WIPP thermodynamic database.

This Analysis Plan (AP) is part of an effort to calculate Pitzer parameters for the interactions of iron (II), lead, and sulfide species with the major components present in the WIPP brines. Experimental data being collected under Test Plan TP 08-02, Iron, Lead, and Sulfide Solubilities, will be used to provide the inputs for this analysis.

The purpose of the analytical work described in this analysis plan is to utilize the data obtained from the experimental work performed in Test Plan TP 08-02, as well as other solubility data in the literature, as inputs to derive thermodynamic properties including Pitzer interaction parameters. Using the NONLIN package, and/or the minimization routine written as a Python script coupled with EQ3/6 Version 8.0a, we will derive various parameters for the different sets of species from the relevant experimental data.

The thermodynamic properties obtained will be incorporated into the WIPP EQ3/6 database for the Pitzer model (i.e., DATA0.FM1). The updated WIPP thermodynamic database, in addition to the current modeling capacities, will enable us to model the interaction of the WIPP brines with iron(II), lead, and sulfide, and will provide an improved model for the solution chemistry in the WIPP repository. Therefore, this study is considered a compliance decision analysis.

1.2 Objectives

The objective of this AP is to derive thermodynamic properties of iron(II), lead, and sulfide species. The thermodynamic properties to be derived include dimensionless standard chemical potentials (\(\mu^o/RT\))/equilibrium constants and Pitzer interaction parameters, at 25°C and 1 bar.
2 Approach

To achieve the objectives of this AP two software programs, either NONLIN or the Python script coupled with EQ3/6 (see following Project Resources), will be used, depending on what data are available. Both of these programs employ inverse fitting methods to obtain the best-fit parameters, and accomplish this by minimizing the difference between the experimental data and the model response.

2.1 Project Resources

Sandia National Laboratories has developed a computer program called NONLIN (Version 2.00, Babb, 1996; Version 2.01, Ismail, 2008). NONLIN fits parameters for the Pitzer’s aqueous electrolyte model based on experimental data for stability constants of aqueous complexes, mineral solubility for a simple system with less than, or equal to, \( \leq \) eight species, osmotic coefficients, electromotive force (e.m.f.), ion exchange data, and solvent extraction. Therefore, this computer program is suitable to achieving the objectives of this AP. In modeling stability constants, osmotic coefficients, e.m.f. data, ion exchange data, and solvent extraction, as a function of ionic strength, the NONLIN code needs to be used. In the manual for NONLIN, there are numerous examples of how to model experimental data. Notice that for solubility data, if there are more than one species contributing to the target total solubility, the solubility data have to be speciated before modeling. For example, if one has the total lead solubility data with PbO being a controlling phase in a NaCl medium, the total lead solubility data need to be speciated as Pb\(^{2+}\), PbCl\(^{+}\), PbCl\(_2\)(aq), and PbCl\(_3\)\(^{–}\) using the relevant conditional stability constants for PbCl\(^{+}\), PbCl\(_2\)(aq), and PbCl\(_3\)\(^{–}\) before modeling.

In addition, there is a Python minimization script (EQ3CodeModule.py) that can be coupled with EQ3NR calculations in the EQ3/6 Version 8.0a (Kirchner, 2012). In this minimization routine, the target thermodynamic parameter can be adjusted to minimize the difference, or to achieve reasonable difference, between the experimental value and predicted value. This minimization routine also can be used to minimize the saturation index by adjusting the target thermodynamic parameters. In this way, the target thermodynamic parameter can be derived. This minimization script is also suitable for achieving the objectives of this AP. In the user’s manual written by Kirchner (2012), there are several examples showing how to obtain the optimized solubility constant by using the script. The Python script coupled with the EQ3/6 Version 8.0a is to be used for evaluation of solubility data to derive Pitzer parameters as well as equilibrium constants.

2.2 Method

The strategy in deriving thermodynamic properties is as follows. If the thermodynamic quantities of the experimental system at reference state are well known, the experimental data will be modeled as a function of ionic strength to derive Pitzer parameter(s) only. If one of the thermodynamic quantities of the experimental system at reference state, for instance, the solubility constant, is less well known, the experimental data will be modeled as a function of ionic strength to derive both the Pitzer parameter(s) and dimensionless standard chemical potential/equilibrium constant of the less well known thermodynamic quantity.
In the Pitzer model, “the $\beta^{(1)}$ parameter has its greatest effect on data modeling in the dilute region” (Choppin et al., 2001). Our experiments are conducted mainly in the high ionic strength region. For instance, the average minimum stoichiometric ionic strength for Tasks 1-2, 5-7, and 10-13, is 0.35 m. As our experimental data are mainly in the high ionic strength region, we follow the paradigm of Choppin et al. (2001) by setting $\beta^{(1)}$ to the average values for certain interactions (Table 1) in order to adjust other parameters. In the work of Choppin et al. (2001), binary interaction parameters include $\beta^{(0)}$, $\beta^{(1)}$ and $C^\phi$.

In addition, in modeling, if the initial modeling returns a large negative value for $\beta^{(0)}$ and a large positive value for $C^\phi$ relative to the literature values for similar complexes, or vice versa, it may indicate that the $C^\phi$ parameter is redundant, and should be set to zero. The $C^\phi$ parameter is the third virial coefficient, and its value is usually very small except for high charge electrolytes such as 4-1/1-4 and 5-1/1-5 electrolytes (Pitzer, 1973; Pitzer and Mayorga, 1973). However, there might be rare instances where the acceptance criteria (below) are not met, or unrealistic values for $\beta^{(0)}$ are obtained when $\beta^{(1)}$ is set to a constant value and $C^\phi$ is set to zero, in these special cases, and at the discretion of the analyst, all three of the Pitzer parameters ($\beta^{(0)}$, $\beta^{(1)}$ and $C^\phi$) could be fit. In documents reporting the results from these special cases, these parameters should be commented with regard to the literature values.

In Choppin et al. (2001), the average $\beta^{(1)}$ parameter for 2:2 interaction is not calculated. In the case where a 2:2 interaction needs to be modeled in a task, the average $\beta^{(1)}$ parameter of 3.27 calculated from Mg$^{2+}$—SO$_4^{2-}$ and Ca$^{2+}$—SO$_4^{2-}$ in the DATA0.FM1 database, coupled with adjusting $\beta^{(0)}$, $\beta^{(2)}$, and $C^\phi$, can be used.

For most interactions, as those listed in Table 1, $\alpha_1$ is 2.0, along with a default value of 12.0 for $\alpha_2$, in the DATA0.FM1 database. As long as $\beta^{(2)}$ is zero, $\alpha_2$ will not be materialized (i.e., $\alpha_2$ is equivalent to zero when the EQ3/6 runs calculations). In most cases, $\beta^{(2)}$ is zero for interactions involving univalent ions. Non-zero $\beta^{(2)}$ is more common for 2:2, 2:3, 3:3, 2:4, and 2:5 interactions for accounting for ion pair association in the dilute range. The average $\beta^{(2)}$ parameter for 2:2 interaction is calculated to be –45.74 based on those for Mg$^{2+}$—SO$_4^{2-}$ and Ca$^{2+}$—SO$_4^{2-}$ interactions in the DATA0.FM1 database. For 2:2, 2:3, 3:3, and 2:4 interactions, $\alpha_1 = 1.4$, and $\alpha_2 = 12.0$, with a non-zero value for $\beta^{(2)}$ (Wolery and Jarek, 2003). For a 2:5 interaction, $\alpha_1 = 1.4$, and $\alpha_2 = 50.0$, with a non-zero value for $\beta^{(2)}$ (Al Mahamid et al., 1998). However, in our experimental systems, the most likely interactions are those listed in Table 1 with some 2:2 interactions.

Table 1. Average $\beta^{(1)}$ parameter for various interactions from Choppin et al. (2001) unless otherwise noted

<table>
<thead>
<tr>
<th>Ion Combination/Interaction Type</th>
<th>$\beta^{(1)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$M^+$, $X^-$; 1:1 interaction</td>
<td>0.29</td>
</tr>
<tr>
<td>$M^+$, $X^-$, and $M^{2+}$, $X^-$; 1:2, 2:1 interaction</td>
<td>1.74</td>
</tr>
<tr>
<td>$M^+$, $X^-$, and $M^{3+}$, $X^-$; 1:3, 3:1 interaction</td>
<td>5.22</td>
</tr>
<tr>
<td>$M^+$, $X^-$, and $M^{4+}$, $X^-$; 1:4, 4:1 interaction</td>
<td>11.6</td>
</tr>
<tr>
<td>$M^{2+}$, $X^{2-}$; 2:2 interaction</td>
<td>3.27*</td>
</tr>
</tbody>
</table>

* calculated from Mg$^{2+}$—SO$_4^{2-}$ and Ca$^{2+}$—SO$_4^{2-}$ interactions; please see the text for details.
The results obtained from running either NONLIN or the Python script will be evaluated and must meet the following acceptance criteria:

1) The fitted values of the Pitzer parameters should be of a similar magnitude compared to those in the peer reviewed literature for comparable interaction types. Many of these Pitzer parameters for these interactions may be found in the thermodynamic databases already in the WIPP records center, DATA0.FM1, DATA0.PIT, and DATA0.YPF. The absolute values of fitted parameters should usually be not larger than the absolute values in the literature by one magnitude. The reference to the literature values should be cited in documents reporting the results.

2) The differences between the measured data and the modeled predictions, e.g., the residuals, should form a curve that has a well-defined minimum when plotted versus the parameter values. The selected “best fit” parameters must correspond to the minimum, or are close to the minimum, in agreement with the first criterion.

3) Visual inspection of the model response using the best fit parameters in comparison with the experimental data demonstrates that they are in close agreement. Graphs showing such comparisons should be included in documents reporting the results.

2.3 Project Tasks and Milestones

There are three major tasks in this AP: (1) computation of solubility constants from experimental data; (2) computation of formation constants from experimental data; and (3) derivation of Pitzer parameters from experimental data. The specific project tasks are detailed in Section 4. The majority of the tasks identified in this AP are planned to be completed by the end of Calendar year 2013, and the milestones for each individual task are specified in Section 4.

3 Software List

The software to be used are NONLIN Version 2.01 (system configuration: OpenVMS 8.2 hp AlphaServer ES47); EQ3/6 Version 8.0a with execution platforms with Microsoft Windows 95, 98, 2000, NT4, XP, Vista, and Window 7; and the Python minimization script tested under the execution platform of EPD_Py25V4.3.0, where EPD stands for Enthought Python Distribution.

4 Tasks

The tasks of this AP are listed below, and milestones for each task are tabulated in Table 2:

(1) Derivation of thermodynamic properties of the system Fe(OH)$_2$-NaCl-Na$_2$SO$_4$-H$_2$O. There are three subtasks in this task: Subtask One—Determination of solubility constant of Fe$_2$O(OH)$_3$Cl(cr); Subtask Two—Derivation of Pitzer mixing parameter of $\theta_{Na^+, Fe^{2+}}$; and Subtask Three—Derivation of Pitzer binary parameter for the interaction between FeOH$^+$ and the bulk electrolyte, NaCl + Na$_2$SO$_4$. 
(2) Derivation of Pitzer binary parameters for the interaction between FeOH$^+$ and the bulk electrolyte, NaCl + Na$_2$CO$_3$.

(3) Derivation of Pitzer binary parameters for the interaction between FeOH$^+$ and the bulk electrolyte, NaHS + Na$_2$S.

(4) Derivation of Pitzer binary parameters for the interaction between Fe$^{2+}$ and the bulk electrolyte, Na$_2$S.

(5) Derivation of Pitzer binary parameters for the interaction between Fe(OH)$_3$ and the bulk electrolyte, NaCl, using oversaturation experiments.

(6) Derivation of Pitzer binary parameters for the interaction between Fe(OH)$_3$ and the bulk electrolyte, CaCl$_2$. This is also to be used as an analog for the interaction between Mg$^{2+}$ and Fe(OH)$_3$.

(7) Derivation of Pitzer parameter for the interaction between neutral species FeOx(aq) and the cation of the bulk electrolyte, NaCl.

(8) Derivation of Pitzer parameter for the interaction between neutral species FeOx(aq) and the cation of the bulk electrolyte, MgCl$_2$.

(9) Derivation of Pitzer parameter for the interaction between neutral species FeOx(aq) and the anion of the bulk electrolyte, NaCl/MgCl$_2$.

(10) Derivation of Pitzer binary parameters for the interaction between FeEDTA$^{2-}$ and the bulk electrolyte, NaCl.

(11) Derivation of Pitzer binary parameters for the interaction between FeEDTA$^{2-}$ and the bulk electrolyte, MgCl$_2$.

(12) Derivation of Pitzer binary parameters for the interaction between FeCit$^-$ and the bulk electrolyte, NaCl.

(13) Derivation of Pitzer binary parameters for the interaction between FeCit$^-$ and the bulk electrolyte, MgCl$_2$.

(14) Derivation of Pitzer binary parameters for the interaction between PbCl$^+$ and the bulk electrolyte, NaCl + NaHCO$_3$.

(15) Derivation of Pitzer binary parameters for the interaction between PbCl$^+$ and the bulk electrolyte, NaCl + Na$_2$CO$_3$.

(16) Derivation of Pitzer binary parameters for the interaction between PbCl$^+$ and the bulk electrolyte, NaCl + Na$_2$SO$_4$.

(17) Derivation of Pitzer binary parameters for the interaction between PbCl$^+$ and the bulk electrolyte, NaCl + NaHS.

(18) Derivation of Pitzer binary parameters for the interaction between PbEDTA$^{2-}$ and the bulk electrolyte, NaCl + Mg$_2$EDTA.

(19) Derivation of Pitzer binary parameters for the interaction between PbEDTA$^{2-}$ and the bulk electrolyte, MgCl$_2$ + Na$_2$H$_2$EDTA.

(20) Derivation of Pitzer binary parameters for the interaction between PbCit$^-$ and the bulk electrolyte, NaCl + MgHCit.

(21) Derivation of Pitzer binary parameters for the interaction between PbCit$^-$ and the bulk electrolyte, MgCl$_2$ + MgHCit.

(22) Derivation of Pitzer binary parameters for the interaction between PbOx(aq) and the bulk electrolyte, NaCl.

(23) Derivation of Pitzer binary parameters for the interaction between PbOx(aq) and the bulk electrolyte, MgCl$_2$.

(24) Derivation of Pitzer binary parameters for the interaction between PbOx(aq) and the bulk electrolyte, NaCl + MgCl$_2$. 
(25) Derivation of Pitzer binary parameters for the interaction between $\text{Na}^+$ and the bulk electrolyte, NaHS.
(26) Derivation of Pitzer binary parameters for the interaction between $\text{Mg}^{2+}$ and the bulk electrolyte, NaHS + Na$_2$S.
(27) Derivation of Pitzer binary parameters for the interaction between $\text{HS}^-$ and the bulk electrolyte, NaCl.
(28) Derivation of Pitzer binary parameters for the interaction between $\text{CaCt}^-$ and the bulk electrolyte, NaCl.
(29) Derivation of Pitzer binary parameters for the interaction between HEDTA$^{3-}$ and the bulk electrolyte, NaCl.
(30) Derivation of Pitzer binary parameters for the interaction between HEDTA$^{3-}$ and the bulk electrolyte, MgCl$_2$.
(31) Determination of solubility constant of di-calcium ethylenediaminetetraacetic acid (Ca$_2$EDTA), Ca$_2$C$_{10}$H$_{12}$N$_2$O$_8$(s)
(32) Determination of stability constant of CaOxalate(aq) in NaCl, MgCl$_2$ solutions and mixtures of NaCl and MgCl$_2$
(33) Derivation of Pitzer mixing parameter of Cl$^-$—FeEDTA$^{2-}$ in NaCl solutions
(34) Derivation of Pitzer mixing parameter of Na$^+$—FeOH$^+$ in NaCl solutions
<table>
<thead>
<tr>
<th>Task</th>
<th>Description</th>
<th>Responsible Individuals</th>
<th>Estimated Completion Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Determination of solubility constant of Fe$_2$(OH)$_3$Cl$_2$(cr)</td>
<td>Nemer/Xiong/Ismail*/Jang</td>
<td>Completed (see Nemer et al., 2010)</td>
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<td>Derivation of $\theta_{\text{Na}^+.,\text{Fe}^{2+}}$</td>
<td>Nemer/Xiong/Ismail*/Jang</td>
<td>Completed (see Nemer et al., 2010)</td>
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<td></td>
<td>Derivation of Pitzer binary interaction parameter of FeOH$^++$—SO$_4^{2-}$</td>
<td>Jang/Kim/Xiong</td>
<td>09/30/2013</td>
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<td>2</td>
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<td>09/30/2013</td>
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<td>Derivation of Pitzer binary interaction parameter of FeOH$^+-HS^-$</td>
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<td>4</td>
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<td>6</td>
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<td>Derivation of Pitzer $\lambda$ parameter of Na$^+$—FeOx(aq)</td>
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<td>Initial Analysis Performed (see Jang, 2012a)</td>
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<td>8</td>
<td>Derivation of Pitzer $\lambda$ parameter of Mg$^{2+}$—FeOx(aq)</td>
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<td>09/30/2014</td>
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<tr>
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<td>Derivation of Pitzer binary interaction parameter of Mg(^{2+})—HS(^-)</td>
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<td>09/30/2014</td>
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<tr>
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<td>Derivation of Pitzer binary interaction parameter of Na(^+)—CaCit(^-)</td>
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<td>Task</td>
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<td>Responsible Individuals</td>
<td>Estimated Completion Date</td>
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<td>Derivation of Pitzer binary interaction parameter of Na(^+)—HEDTA(^3-)</td>
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<td>Derivation of Pitzer binary interaction parameter of Mg(^{2+})—HEDTA(^3-)</td>
<td>Xiong</td>
<td>12/31/2013</td>
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<td>31</td>
<td>Determination of solubility constant of di-calcium ethylenediaminetetraacetic acid (Ca(<em>2)EDTA), Ca(<em>2)C(</em>{10})H(</em>{12})N(_2)O(_8)(s)</td>
<td>Xiong</td>
<td>Completed (see Xiong, 2012)</td>
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<td>32</td>
<td>Determination of stability constant of CaOxalate(aq)</td>
<td>Jang</td>
<td>09/30/2014</td>
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<td>Derivation of Pitzer mixing parameter of Cl(^-)—FeEDTA(^2-)</td>
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<td>Derivation of Pitzer mixing parameter of Na(^+)—FeOH(^+)</td>
<td>Jang</td>
<td>09/30/2014</td>
</tr>
</tbody>
</table>

* A.E. Ismail is no longer working for Sandia National Laboratories.

5 **Special Considerations**

The thermodynamic properties including Pitzer interaction parameters derived in this AP will be summarized in memos/analysis reports that will be submitted to the WIPP Record Center.

6 **Applicable Procedures**

All applicable WIPP QA procedures will be followed when conducting this AP.
- Training of personnel will be conducted in accordance with the requirements of NP 2-1, *Qualification and Training*.
- Analyses will be conducted and documented in accordance with the requirements of NP 9-1, *Analyses*.
- All software used will meet the requirements laid out in NP 19-1, *Software Requirements* and NP 9-1, as applicable.
- The analyses will be reviewed following NP 6-1, *Document Review Process*.
- All required records will be submitted to the WIPP Records Center in accordance with NP 17-1, *Records*. 
7 References


Xiong, Y.-L., 2012. “Experimental determination of solubility constant of di-calcium ethylenediaminetetraacetic acid (Ca_2EDTA), Ca_2C_{10}H_{12}N_2O_8(s), in the NaCl–H_2O system”, Analysis Report for AP-154. Carlsbad, NM: Sandia National Laboratories. ERMS 558669.
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