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Sandia National Laboratories

Je-Hun Jang
4100 National Parks Highway
Carlsbad, NM 88220
Phone: (505) 284-2770
Fax: (575) 234-0061
E-mail: jjang@sandia.gov

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To: Records Center

From: Je-Hun Jang

Subject: Derivation of Pitzer ion interaction parameters for the pair $Na^+$ and $FeEDTA^{2-}$

This memo is written to describe the derivation of Pitzer interaction parameters for the pair of $Na^+$ and $FeEDTA^{2-}$. This derivation is associated with Test Plan TP 08-02 , "Iron, Lead, Sulfide, and EDTA Solubilities" (Ismail et al., 2008) and Analysis Plan AP-154, "Analysis Plan for Derivation of Thermodynamic Properties Including Pitzer Parameters for Solubility Studies of Iron, Lead and EDTA", Task 10 in Table 1 therein (Xiong, 2011a). Briefly, an aqueous model for dissolution of $Fe(OH)_2(s)$ in mixed $Na_2H_2EDTA$ and NaCl solution was fitted to the experimentally measured solubility data. The aqueous model consists of several chemical reactions and related Pitzer interaction parameters (See section 4 below for details). The model is implemented within the aqueous speciation code EQ3/6 v.8.0a (Wolery and Jarek, 2003). Specifically, Pitzer binary interaction parameters for the $Na^+$ and $FeEDTA^{2-}$ pair ($\beta^{(0)}$, $\beta^{(1)}$, and $C^{\phi}$; Table 5) were fitted to the experimental data (Table 3).

EQ3NR packaged in EQ3/6 v.8.0a was used to calculate the aqueous speciation and saturation index for a given number of EQ3NR input files (*.3i files). A *.3i file represents one set of measurements from an individual experiment. To calculate the aqueous speciation and saturation index, EQ3NR refers to one of the databases (e.g., data0.fm1) for values of logK's (10-based logarithm of equilibrium constants for reactions) and Pitzer parameters. The saturation index indicates how far the system is from equilibrium with respect to the solid of interest, and can be calculated from the aqueous speciation. The value could be (i) zero if the system is saturated (equilibrated) with the solid of interest, (ii) positive if the system is supersaturated with the solid of interest, or (iii) negative if the system is undersaturated with the solid of interest. Thus, the smaller the sum of squared saturation indices that the aqueous model calculates for the given number of *.3i files, the more closely the model attributes equilibrium to the individual experiment with respect to the solid of interest.

Hence, we seek $\beta^{(0)}$, $\beta^{(1)}$, and $C^{\phi}$ (Table 5) that make the sum of squared saturation indices as small as possible. To do so, the calculation of aqueous speciation and saturation index was repeated by adjusting the $\beta^{(0)}$, $\beta^{(1)}$, and $C^{\phi}$ in the database (e.g., data0.fm1) until the values of $\beta^{(0)}$, $\beta^{(1)}$, and $C^{\phi}$ were found that make the sum of squared saturation indices the least for the given number of *.3i files. The repetition was driven by a script written in the Python computer language, *EQ3CodeModule.py* (Kirchner, 2012).

1. Experimental data for the fitting

Experimental data used in this analysis is summarized in Table 1 below. The values are from Table 3-18 in Jang et al. (2012).

Table 1. Experimental data for derivation of $\beta^{(0)}$, $\beta^{(1)}$, and $C^{\Phi}$ for the pair of $FeEDTA^{2-}$ and $Na^{+}$.

| Experiment ID | Na(I) (M) | $EDTA^{4-}$ (M) | pH | Fe(II)[a] (M) |
|---|---|---|---|---|
| Fe(OH)2-Na4EDTA-0.01A | 9.48E-02 | 4.09E-02 | 7.820 | 5.31E-02 |
| Fe(OH)2-Na4EDTA-0.1A | 1.59E-01 | 3.92E-02 | 7.948 | 4.73E-02 |
| Fe(OH)2-Na4EDTA-1A | 8.09E-01 | 4.04E-02 | 8.265 | 3.81E-02 |
| Fe(OH)2-Na4EDTA-2A | 1.58E+00 | 4.02E-02 | 8.593 | 3.76E-02 |
| Fe(OH)2-Na4EDTA-3A | 2.37E+00 | 4.12E-02 | 8.729 | 3.69E-02 |
| Fe(OH)2-Na4EDTA-4A | 2.78E+00 | 3.96E-02 | 8.766 | 3.31E-02 |
| Fe(OH)2-Na4EDTA-5A | 3.40E+00 | 4.02E-02 | 8.930 | 3.40E-02 |
| Fe(OH)2-Na4EDTA-0.01B | 9.31E-02 | 3.97E-02 | 7.847 | 5.01E-02 |
| Fe(OH)2-Na4EDTA-0.1B | 1.62E-01 | 3.98E-02 | 7.921 | 4.83E-02 |
| Fe(OH)2-Na4EDTA-1B | 8.26E-01 | 3.93E-02 | 8.341 | 3.90E-02 |
| Fe(OH)2-Na4EDTA-2B | 1.61E+00 | 3.95E-02 | 8.481 | 3.74E-02 |
| Fe(OH)2-Na4EDTA-3B | 2.23E+00 | 3.99E-02 | 8.730 | 3.64E-02 |
| Fe(OH)2-Na4EDTA-4B | 3.01E+00 | 3.96E-02 | 8.849 | 3.48E-02 |
| Fe(OH)2-Na4EDTA-5B | 3.25E+00 | 4.03E-02 | 8.928 | 3.33E-02 |

[a] Measured by ICP-AES assuming [Fe(II)] = Total dissolved Fe concentration ($[Fe_T]$). [ ] denotes molar concentrations.

2. Data conversion

Input files for EQ3NR run require data to be in molal (m) unit. Thus, data given in molar (M) unit was converted to molal (m) unit by applying the ratio of M to m (M_m, in the unit of kg.$H_2O$/L.solution, Table 2).

The pH values in Table 1 are those measured by pH electrodes and meters, which are typically calibrated with respect to pH buffers of low ionic strength. Therefore, to account for the bias introduced by higher ionic strength used in the experiments, the value should be converted to $pC_{H^+}$ (negative 10-based logarithm of molar concentration of $H^+$) using the correction factor defined for NaCl-dominated brines ($A_{NaCl}$) in Roselle (2011). :

$$A_{NaCl}\ (\pm 0.47) = 0.186 \cdot I_M - 0.105 \qquad \text{(ii)}$$

$$pC_{H^+} = pH + A_{NaCl} \qquad \text{(iii)}$$

where $I_M$ is molar ionic strength of the solution.

Negative 10-based logarithm of molal concentration of $H^+$ (pmH in Table 3 below) can be calculated from $pC_{H^+}$ by equation below:

$$pmH = -\log[10^{-pC_{H^+}}/(M\_m)] \qquad \text{(iv)}$$

Values for $A_{NaCl}$ and M_m as a function of ionic strength are summarized in Table 2.

Table 2. Ionic strength, $A_{NaCl}$, solution density, and M_m[d].

| Experiment ID | [Cl(-I)][a] | $I_M$[b] | $A_{NaCl}$ | ρ[c] | M_m[d] |
|---|---|---|---|---|---|
| Fe(OH)2-Na4EDTA-0.01A | 1.30E-02 | 0.381 | -0.034 | 1.0184 | 1.004 |
| Fe(OH)2-Na4EDTA-0.1A | 8.06E-02 | 0.433 | -0.024 | 1.0071 | 0.989 |
| Fe(OH)2-Na4EDTA-1A | 7.28E-01 | 1.092 | 0.098 | 1.0360 | 0.980 |
| Fe(OH)2-Na4EDTA-2A | 1.50E+00 | 1.861 | 0.241 | 1.0757 | 0.975 |
| Fe(OH)2-Na4EDTA-3A | 2.29E+00 | 2.658 | 0.389 | 1.1035 | 0.956 |
| Fe(OH)2-Na4EDTA-4A | 2.70E+00 | 3.057 | 0.464 | 1.1326 | 0.962 |
| Fe(OH)2-Na4EDTA-5A | 3.32E+00 | 3.681 | 0.580 | 1.1409 | 0.933 |
| Fe(OH)2-Na4EDTA-0.01B | 1.37E-02 | 0.371 | -0.036 | 1.0184 | 1.004 |
| Fe(OH)2-Na4EDTA-0.1B | 8.24E-02 | 0.441 | -0.023 | 1.0071 | 0.989 |
| Fe(OH)2-Na4EDTA-1B | 7.47E-01 | 1.101 | 0.100 | 1.0360 | 0.979 |
| Fe(OH)2-Na4EDTA-2B | 1.53E+00 | 1.887 | 0.246 | 1.0757 | 0.973 |
| Fe(OH)2-Na4EDTA-3B | 2.15E+00 | 2.509 | 0.362 | 1.1035 | 0.965 |
| Fe(OH)2-Na4EDTA-4B | 2.93E+00 | 3.287 | 0.506 | 1.1326 | 0.948 |
| Fe(OH)2-Na4EDTA-5B | 3.17E+00 | 3.532 | 0.552 | 1.1409 | 0.942 |

[a] Chloride concentration was calculated: [Na(I)] - 2×[$EDTA^{4-}$], since solution was made from NaCl and $Na_2H_2EDTA.2H_2O$. [ ] denotes molar concentrations.

[b] Molar ionic strength ($I_M$) = $0.5\times([Na(I)]\times(+1)^2 + [EDTA^{4-}]\times(-4)^2 + [Cl(-I)]\times(-1)^2)$.

[c] ρ denotes solution density in g/mL or, equivalently, kg/L. Source: WIPP-Solubility-31, p.16.

[d] M_m denotes Molar-to-molal conversion factor in the unit of kg.$H_2O$/L.solution.

3. Data used in the fitting

Using the conversion factors in Table 2, the experimental data in Table 1 were converted to numbers in molal (m) unit, which are to be used in the model fitting.

Table 3. Experimental data to be used in the model fitting (in molal unit) and corresponding EQ3NR input files (*.3i).

| Experiment ID | Na(I) | $\Sigma EDTA^{4-}$ | Cl(-I) | Fe(II) | pmH | filename |
|---|---|---|---|---|---|---|
| Fe(OH)2-Na4EDTA-0.01A | 9.44E-02 | 4.07E-02 | 1.29E-02 | 5.29E-02 | 7.788 | edna01.3i |
| Fe(OH)2-Na4EDTA-0.1A | 1.61E-01 | 3.96E-02 | 8.15E-02 | 4.78E-02 | 7.919 | edna02.3i |
| Fe(OH)2-Na4EDTA-1A | 8.26E-01 | 4.12E-02 | 7.43E-01 | 3.89E-02 | 8.354 | edna03.3i |
| Fe(OH)2-Na4EDTA-2A | 1.62E+00 | 4.12E-02 | 1.54E+00 | 3.86E-02 | 8.823 | edna04.3i |
| Fe(OH)2-Na4EDTA-3A | 2.48E+00 | 4.31E-02 | 2.39E+00 | 3.86E-02 | 9.099 | edna05.3i |
| Fe(OH)2-Na4EDTA-4A | 2.89E+00 | 4.12E-02 | 2.81E+00 | 3.44E-02 | 9.213 | edna06.3i |
| Fe(OH)2-Na4EDTA-5A | 3.64E+00 | 4.31E-02 | 3.56E+00 | 3.64E-02 | 9.480 | edna07.3i |
| Fe(OH)2-Na4EDTA-0.01B | 9.27E-02 | 3.95E-02 | 1.36E-02 | 4.99E-02 | 7.813 | edna08.3i |
| Fe(OH)2-Na4EDTA-0.1B | 1.64E-01 | 4.02E-02 | 8.33E-02 | 4.88E-02 | 7.893 | edna09.3i |
| Fe(OH)2-Na4EDTA-1B | 8.44E-01 | 4.01E-02 | 7.63E-01 | 3.98E-02 | 8.432 | edna10.3i |
| Fe(OH)2-Na4EDTA-2B | 1.65E+00 | 4.06E-02 | 1.57E+00 | 3.84E-02 | 8.715 | edna11.3i |
| Fe(OH)2-Na4EDTA-3B | 2.31E+00 | 4.14E-02 | 2.23E+00 | 3.77E-02 | 9.076 | edna12.3i |
| Fe(OH)2-Na4EDTA-4B | 3.17E+00 | 4.18E-02 | 3.09E+00 | 3.67E-02 | 9.332 | edna13.3i |
| Fe(OH)2-Na4EDTA-5B | 3.45E+00 | 4.28E-02 | 3.36E+00 | 3.53E-02 | 9.454 | edna14.3i |

4. Model description

Aqueous model consists of aqueous reactions, dissolution reactions, and related Pitzer interaction parameters. Reactions are summarized in Table 4 and Pitzer parameters in Table 5.

Table 4. Reactions and 10-based logarithms of their equilibrium constants (logK's) used in this model fitting.

| Reactions | logK | Source |
|---|---|---|
| Aqueous reactions | | |
| (1) $H^+ + OH^- = H_2O$ | 13.9967 | data0.fm1[a] |
| (2) $H_4EDTA(aq) = 4H^+ + EDTA^{4-}$ [b] | -23.0393 | data0.fm1 |
| (3) $H_3EDTA^- = 3H^+ + EDTA^{4-}$ | -20.5374 | data0.fm1 |
| (4) $H_2EDTA^{2-} = 2H^+ + EDTA^{4-}$ | -17.4500 | data0.fm1 |
| (5) $HEDTA^{3-} = H^+ + EDTA^{4-}$ | -10.5707 | data0.fm1 |
| (6) $FeOH^+ + H^+ = Fe^{2+} + H_2O$ | 9.3148 | data0.ymp.R2[c] |
| (7) $FeEDTA^{2-} = Fe^{2+} + EDTA^{4-}$ | -16.1 | Morel and Hering (1993) |
| Dissolution | | |
| (8) $Fe(OH)_2(s) + 2H^+ = Fe^{2+} + 2H_2O$ | 12.95 | Nemer et al. (2011) |
| (9) $NaCl(s) = Na^+ + Cl^-$ | 1.5704 | data0.fm1 |

[a] data0.fm1: See Xiong (2011b)

[b] $EDTA^{4-}$: $C_{10}H_{12}O_8N_2^{4-}$

[c] data0.ymp.R2 is one of the EQ3/6 databases that come within the installation package for EQ3/6 v.8.0a.

Table 5. Pitzer interaction parameters used in this model fitting. Three Pitzer parameters for $FeEDTA^{2-}$ /$Na^+$ pair ($\beta^{(0)}$, $\beta^{(1)}$, and $C^{\phi}$) were fitted to the experimental data in this memo.

| *i* | *j* | $\beta^{(0)}$ | $\beta^{(1)}$ | $\beta^{(2)}$ | $C^{\phi}$ | Source |
|---|---|---|---|---|---|---|
| $Na^+$ | $Cl^-$ | 0.0765 | 0.2664 | - | 0.00127 | data0.fm1[a] |
| $Na^+$ | $OH^-$ | 0.0864 | 0.253 | - | 0.0044 | data0.fm1 |
| $Na^+$ | $H_3EDTA^-$ | -0.2345 | 0.29 | - | 0.059 | data0.fm1 |
| $Na^+$ | $H_2EDTA^{2-}$ | -0.1262 | 1.74 | - | 0.054 | data0.fm1 |
| $Na^+$ | $HEDTA^{3-}$ | 0.5458 | 5.22 | - | -0.048 | data0.fm1 |
| $Na^+$ | $EDTA^{4-}$ | 1.016 | 11.6 | - | 0.001 | data0.fm1 |
| $H^+$ | $Cl^-$ | 0.1775 | 0.2945 | - | 0.0008 | data0.fm1 |
| $Fe^{2+}$ | $Cl^-$ | 0.3359 | 1.5322 | - | -0.00861 | Pitzer and Mayorga (1973) |
| $Na^+$ | $FeEDTA^{2-}$ | TBD[b] | TBD[b] | - | TBD[b] | This memo |

| *i* | *j* | $\theta_{cc'}$ or $\theta_{aa'}$ | Source |
|---|---|---|---|
| $Na^+$ | $H^+$ | 0.036 | data0.fm1 |
| $Na^+$ | $Fe^{2+}$ | 0.08 | Nemer et al. (2011) |
| Cl- | $OH^-$ | -0.05 | data0.fm1 |

| *i* | *j* | *k* | $\psi_{cc'a}$ or $\psi_{aa'c}$ | Source |
|---|---|---|---|---|
| $Na^+$ | $H^+$ | $Cl^-$ | -0.004 | data0.fm1 |
| Cl- | $OH^-$ | $Na^+$ | -0.006 | data0.fm1 |

[a] data0.fm1: See Xiong (2011b)
[b] TBD: To Be Determined

5. Text blocks required to update an EQ3/6 database (e.g., data0.fm1) for the model fitting

The following eight text blocks should be copied to appropriate places in an EQ3/6 database (e.g., data0.fm1) for the model fitting described in this memo.

5.1. Elemental iron.

The line below should be inserted under "elements" section of an EQ3/6 database (Domski, 2012).

```
Fe          55.84500
```

5.2. Block to add ferrous iron cation ($Fe^{2+}$) as a basis species.

The block below defines the ferrous iron cation (Fe++) as a basis species for aqueous speciation calculation. This block should be copied under "basis species" section of an EQ3/6 database (Domski, 2012).

```
+--------------------------------------------------------------------
Fe++
     charge  =   2.0
****
     1 element(s):
      1.0000 Fe
+--------------------------------------------------------------------
```

## 5.3. Block for reaction (6) in Table 4.

The block below addresses the reaction (6) in Table 4. This block should be copied under "aqueous species" section of an EQ3/6 database. The information in this block comes from "data0.ymp.R2", and the extra information therein was trimmed out, so that the format of this block is consistent with that of "data0.fm1". "data0.ymp.R2" is one of the EQ3/6 databases that come within the installation package for EQ3/6 v.8.0a.

```
+------------------------------------------------------------------------
FeOH+                       FeOH+
     charge  =   1.0
****
     3 element(s):
      1.0000 H              1.0000 Fe             1.0000 O
****
     4 species in aqueous dissociation reaction:
    -1.0000  FeOH+                        -1.0000  H+
     1.0000  Fe++                          1.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data     9.3148   No_Data    No_Data
        No_Data    No_Data   No_Data    No_Data
* Source: data0.ymp.R2
+------------------------------------------------------------------------
```

## 5.4. Block for reaction (7) in Table 4.

The block below addresses the reaction (7) in Table 4. This block should be copied under "aqueous species" section of an EQ3/6 database.

```
+------------------------------------------------------------------------
FeEDTA--                    FeC10H12O8N2--
     charge  =  -2.0
****
     5 element(s):
     10.0000 C              12.0000 H             1.0000 Fe
      2.0000 N               8.0000 O
****
     3 species in aqueous dissociation reaction:
    -1.0000  FeEDTA--                    1.0000  Fe++
     1.0000  EDTA----
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data    -16.100   No_Data    No_Data
        No_Data    No_Data   No_Data    No_Data
* Source: -16.1 Morel and Hering (1993), p.339, I=0, 25 degree C
+------------------------------------------------------------------------
```

## 5.5. Block for reaction (8) in Table 4.

The block below addresses the reaction (8) in Table 4. This block should be copied under "solids" section of an EQ3/6 database.

```
+------------------------------------------------------------------------
Fe(OH)2-Hex                 Fe(OH)2
     V0PrTr  =    24.630 cm**3/mol [source: supcrt92 ]
****
     3 element(s):
      2.0000 H              1.0000 Fe             2.0000 O
****
```

```
     4 species in aqueous dissociation reaction:
    -1.0000  Fe(OH)2-Hex                -2.0000  H+
     1.0000  Fe++                        2.0000  H2O
*
**** logK grid [0-25-60-100C @1.0132bar; 150-200-250-300C @Psat-H2O]:
        No_Data    12.9500    No_Data    No_Data
        No_Data    No_Data    No_Data    No_Data
* Source: 12.95, Nemer et al. (2011)
+--------------------------------------------------------------------
```

## 5.6. Block for Pitzer parameters for ion pair of $Fe^{2+}$ and $Cl^-$ in Table 5.

The block below addresses the Pitzer parameters for ion pair of $Fe^{2+}$ and $Cl^-$ in Table 5. This block should be copied under "ca combinations: beta(n)(ca) and Cphi(ca) [optional: alpha(n)(ca)]" section of an EQ3/6 database.

```
+------------------------------------------------------------
Fe++                        Cl-
  alpha(1) = 2.0
  alpha(2) = 12.0
  beta(0)
    a1 = 0.33590
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(1)
    a1 = 1.53220
    a2 = 0.
    a3 = 0.
    a4 = 0.
  beta(2)
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = -0.00861
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Pitzer and Mayorga (1973), Pitzer (1991)
+------------------------------------------------------------
```

## 5.7. Block for Pitzer parameters for ion pair of $Na^+$ and $Fe^{2+}$ in Table 5.

The block below addresses the Pitzer parameters for ion pair of $Na^+$ and $Fe^{2+}$ in Table 5. This block should be copied under "cc' and aa' combinations: theta(cc') and theta(aa')" section of an EQ3/6 database.

```
+------------------------------------------------------------
Na+                         Fe++
  theta:
    a1 = 0.08
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: Nemer et al. (2011)
+------------------------------------------------------------
```

5.8. Block for Pitzer parameters for the pair of $Na^+$ and $FeEDTA^{2-}$ in Table 5.

The block below addresses the Pitzer parameters for the pair of $Na^+$ and $FeEDTA^{2-}$ in Table 5. This block should be copied under "ca combinations: beta(n)(ca) and Cphi(ca) [optional: alpha(n)(ca)]" section of an EQ3/6 database.

```
+--------------------------------------------------------------------
Na+                          FeEDTA--
  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 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
  Cphi:
    a1 = 0.0
    a2 = 0.
    a3 = 0.
    a4 = 0.
* Source: To be estimated in this memo
+--------------------------------------------------------------------
```

6. Results and discussion

Fitting started with running the Python script "FeEDTA_Na.py" and "EQ3CodeModule.py" (listed in section 7.2. below). Fitting results are summarized in Table 6 below.

Table 6. Fitting results.

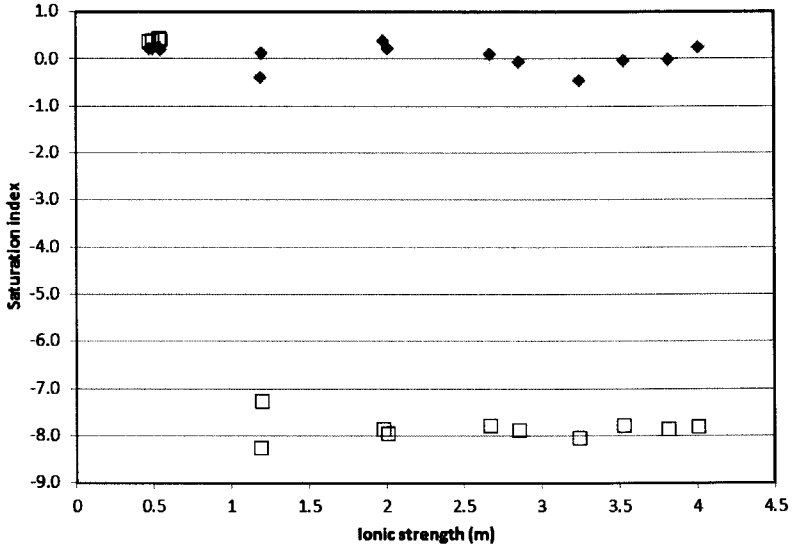
| Pitzer parameters | value | Residual |
|---|---|---|
| $\beta^{(0)}$ | -8.43 | |
| $\beta^{(1)}$ | 52.49 | 0.854 |
| $C^{\phi}$ | 3.41 | |

For those who may want to reproduce in an exact manner the results of this memo using the Python script and EQ3NR input files (*.3i files), $\beta^{(0)}$ = -8.43139547969, $\beta^{(1)}$ = 52.4903986284, and $C^{\phi}$ = 3.41271520133. The minimized sum of squared saturation indices is 0.8539107855.

The values of saturation indices from 14 experiments are confined within a narrow range of -0.463 to 0.390 over the entire ionic strength investigated (Figure 1). This indicates that the aqueous model (Table 4 and 5), including newly fitted $\beta^{(0)}$, $\beta^{(1)}$, and $C^{\phi}$, predicts the equilibria with respect to $Fe(OH)_2(s)$ for all the 14 experiments very closely.

The fitting procedure in this memo was reproduced independently by Paul Domski. See APPENDIX for his email regarding the reproduction of this fitting.

Figure 1. Plot of saturation indices over ionic strength. Blue solid diamonds aligned around 0.0 (within a range of -0.463 to 0.390) represent the saturation indices calculated with fitting of the Pitzer interaction parameters for $Na^+/FeEDTA^{2-}$ pair to the experimental data. Red open squares represent the saturation indices calculated without considering Pitzer interaction in $Na^+/FeEDTA^{2-}$ pair.




7. Files to be submitted

7.1. EQ3NR input files (*.3i, 14 files in total) and output files (*.3o, 14 files in total)

Input files: edna01.3i, edna02.3i, edna03.3i, edna04.3i, edna05.3i, edna06.3i, edna07.3i, edna08.3i, edna09.3i, edna10.3i, edna11.3i, edna12.3i, edna13.3i, edna14.3i.
Output files: edna01.3o, edna02.3o, edna03.3o, edna04.3o, edna05.3o, edna06.3o, edna07.3o, edna08.3o, edna09.3o, edna10.3o, edna11.3o, edna12.3o, edna13.3o, edna14.3o.

7.2. Python scripts

FeEDTA_Na.py (to be copied into the same folder as EQ3NR input files above; this file drives the fitting procedure)
EQ3CodeModule.py (to be copied into either the same folder as EQ3NR input files above or C:\Python27\Lib for versatile access; this file contains Python modules necessary for the fitting)

7.3. Excel files

Pitzer_FeEDTA_Na.xlsx (used for data conversion in Tables 1, 2, and 3)
GetEQData_v101e.xls (contains excel macro that extracts numbers from EQ3NR output files, *.3o)

FeEDTA_Na.xls (contains ionic strength, saturation indices, and their plot, generated using excel macro in the file above)

7.4. Email from Paul Domski on 10/10/2012

RE AP-154 Task 10 FeEDTANa pair.pdf (See APPENDIX for its content)

8. References


Domski, P.S. (2012) Memo to Records Center, Memo AP-154, Task 10 EQ3/6 Database Update. (This reference is cited in APPENDIX below)

Ismail, A.E., M.B. Nemer, G.T. Roselle, and Y.-L. Xiong. 2008. Iron, Lead, Sulfide, and EDTA Solubilities Test Plan, Sandia National Laboratories, TP 08-02. ERMS 548467.

Jang, J.-H., Y.L. Xiong, S. Kim, and M.B. Nemer (2012) Second Milestone Report on Test Plan TP 08-02, "Iron, Lead, Sulfide, and EDTA Solubilities", Sandia National Laboratories, ERMS 557198.

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APPENDIX: Email from Paul Domski to Je-Hun Jang on 10/10/2012

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From: Domski, Paul S
Sent: Wednesday, October 10, 2012 8:04 AM
To: Jang, Je-Hun
Cc: Roselle, Gregory Thomas; Nielsen, Shelly R
Subject: RE: AP-154 Task 10 FeEDTA/Na pair

Je-Hun,

I have independently reproduced the values that you estimated in your memo using the inputs that you provided to me in your draft memo entitled "Memo_Pitzer_FeEDTA_Na.docx". The parameters and values that I estimated using the Python script include the beta(0), beta(1), and C for sodium ion - FeEDTA-- ion pair. The values are as follows: beta(0) = -8.43, beta(1) = 52.49, and C = 3.41 with the residual of 0.854. Note there was a slight difference in the residual that is reported in the memo, 0.853, and value that I got, this has no impact on the estimated parameters.

Paul Domski
S.M. Stoller Corp
(505) 604-6736

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From: Jang, Je-Hun
Sent: Friday, October 05, 2012 2:28 PM
To: Domski, Paul S
Cc: Roselle, Gregory Thomas; Nielsen, Shelly R
Subject: AP-154 Task 10 FeEDTA/Na pair
Paul,

Attached is a zip file that has every components (I guess) you need to do the calculation.
Please let me know if you have any questions.
It feels like fall has come.
Have a nice weekend!!

Je-Hun Jang.

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Note: Memo related to this email is Domski (2012).