

**Thermodynamics of Brines,  
Minerals and Corrosion Products  
at High Temperatures: A Pitzer  
Model for the Na-Al(OH)<sub>4</sub>-Cl-OH  
System to High Ionic Strength and  
to 250°C**

**Fuel Cycle Research & Development**

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*Yongliang Xiong*  
*Sandia National Laboratories*  
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# FCT Quality Assurance Program Document

## Appendix E FCT Document Cover Sheet

Thermodynamics of Brines, Minerals and Corrosion Products at High Temperatures: A Pitzer Model for the Na-Al(OH)<sub>4</sub>-Cl-OH System to High Ionic Strength and to 250°C (M3FT-13SN08180322)

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## SUMMARY

This work is conducted under Task 2.5, *Development of a Chemical Model/database up to 200 °C with High Internal Consistency*, in the TP Test Plan for Determining Thermodynamic Properties of Brines, Minerals and Corrosion Products for High Level Radioactive Waste Disposal in Salt (FCRD-UFD-2012-00033). In this work, a Pitzer model for the Na-Cl-OH-Al(OH)<sub>4</sub> system, and solubility of boehmite (AlOOH) to high ionic strengths, and to high temperatures up to 250°C, has been developed by evaluating equilibrium quotients concerning boehmite in NaCl solutions to 5.0 mol•kg<sup>-1</sup>, and boehmite solubility data in NaOH solutions to ~13 mol•kg<sup>-1</sup>. This model is validated by comparing model-predicted solubilities with solubility data of boehmite in NaOH solutions that are independent from the model development. In combination with the Pitzer parameters for the Na<sup>+</sup>—Al(OH)<sub>4</sub><sup>-</sup> interaction to 100°C recommended by the author, already published in the literature, a Pitzer model concerning aluminum under the neutral to alkaline pH conditions to high ionic strength valid from 25°C to 250°C, has been established. This model is applicable to high level waste (HLW) and used fuel disposal in salt formations in accurate descriptions of geological behavior of aluminum species in brines over a wide range of temperatures. This model, coupled with the high temperature borate and silica models to be developed, will be of use in prediction of stability of HLW borosilicate glass, aluminum silicate materials as waste forms for long-lived nuclides, bentonite as engineered barrier, in geological repositories.

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## ACRONYMS

DOE-NE	The Department of Energy Office of Nuclear Energy
FCRD	Fuel cycle research and development
HLW	High level nuclear waste
m	Concentration on molal scale
R&D	Research and development
TP	Test Plan
UFD	Used fuel disposition
UNF	Used nuclear fuel

# THERMODYNAMICS OF BRINES, MINERALS AND CORROSION PRODUCTS AT HIGH TEMPERATURES: A PITZER MODEL FOR THE $\text{Na-Al(OH)}_4\text{-Cl-OH}$ SYSTEM TO HIGH IONIC STRENGTH AND TO $250^\circ\text{C}$

## 1. OBJECTIVE

Accurate knowledge of geochemical behavior of aluminum in high ionic strength solutions at elevated temperatures is important to safe disposal of high level nuclear waste (HLW) and used nuclear fuel (UNF) in geological repositories, especially in salt formations. The importance of accurate knowledge of geochemical behavior of aluminum is related to the following facts. Borosilicate glasses in which aluminum is a major component are a strong candidate waste form for immobilization of high level nuclear waste (HLW). Sodalite,  $\text{Na}_8(\text{Al}_6\text{Si}_6\text{O}_{24})(\text{OH}, \text{Cl}, \text{I})_2$ , is a candidate waste form for contaminated salt wastes generated from electrorefinery of used nuclear fuel, and for radioactive iodine (i.e.,  $^{129}\text{I}$ ) waste (e.g., Sheppard et al., 2006). Bentonite,  $\text{Na}_{0.2}\text{Ca}_{0.1}\text{Al}_2\text{Si}_4\text{O}_{10}(\text{OH})_2(\text{H}_2\text{O})_{10}$ , is a preferred engineered barrier for HLW and used nuclear fuel in many geological repository designs (e.g., Itälä, 2009).

$\text{Al(OH)}_4^-$  is expected to be a dominant aluminum species from the mildly acidic to alkaline pH at elevated temperatures. For example, the neutral pH is 5.8 at  $150^\circ\text{C}$ , and  $\text{Al(OH)}_4^-$  predominates from  $\text{pH}_m \sim 4$  (hydrogen ion concentration on molal scale) to alkaline  $\text{pH}_m$  in a solution with 1.0 molal ionic strength (Palmer et al., 2001). Wesolowski (1992) recommended two sets of the Pitzer parameters for the  $\text{Na}^+ - \text{Al(OH)}_4^-$  interaction. One set is at  $25^\circ\text{C}$ , and was obtained by using the equations of Pitzer and Mayorga (1973). The other set is at  $0 - 100^\circ\text{C}$ , which was evaluated by using equations of Simonson et al. (1989). The former is adopted in the Al-Si thermodynamic model to  $100^\circ\text{C}$ , assuming the constancy of the Pitzer parameters over  $25 - 100^\circ\text{C}$  (Xiong, 2013). This assumption is in line with the suggestion that Pitzer and SIT parameters can be regarded to be constant over a narrow temperature range (e.g., Grenthe et al., 1997). The latter was adopted by Königsberg et al. (2006) to calculate solubilities of boehmite.

In this work, an attempt is made to evaluate Pitzer parameters for the  $\text{Na}^+ - \text{Al(OH)}_4^-$  interaction in the temperature range from  $100^\circ\text{C}$  to  $250^\circ\text{C}$ , based on the high quality experimental equilibrium quotients involving  $\text{Al(OH)}_4^-$ . Then, experimental solubility data of boehmite in NaOH solutions are used to evaluate the mixing parameters involving  $\text{Al(OH)}_4^-$  to  $170^\circ\text{C}$ . Finally, independent experimental data are compared with model predicted solubilities of boehmite in the same medium.

In combination with the Pitzer parameters for the  $\text{Na}^+ - \text{Al(OH)}_4^-$  interaction to  $100^\circ\text{C}$  (Xiong, 2013), the objective of this work is to establish a Pitzer model concerning aluminum under the neutral to alkaline pH conditions to high ionic strength valid from  $25^\circ\text{C}$  to  $250^\circ\text{C}$ .

This work is conducted under Task 2.5, *Development of a Chemical Model/database up to  $200^\circ\text{C}$  with High Internal Consistency*, in the TP Test Plan for Determining Thermodynamic Properties of Brines, Minerals and Corrosion Products for High Level Radioactive Waste Disposal in Salt (FCRD-UFD-2012-00033; Xiong et al., 2012).



## 2. SCIENTIFIC APPROACH AND TECHNICAL METHODS

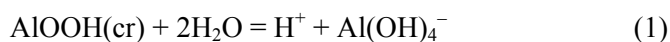
### 2.1 Scientific Approach

In this work, the standard state for a solid phase is defined as its pure end-member with unit activity at temperatures and pressures of interest. The standard state of the solvent in aqueous solutions is pure solvent at temperatures and pressures of interest. The standard state for an aqueous solute is a hypothetical 1 molal (m) solution referred to infinite dilution at temperatures and pressures of interest. The uncertainties reported in this study are two standard deviations ( $2\sigma$ ). Error propagations are calculated based on uncertainties associated with regressions and equilibrium constants in the model.

The computer code EQ3/6 Version 8.0a (Wolery et al., 2010; Xiong, 2011) is employed as the modeling platform. The essence of the modeling is to minimize the difference between experimental and model predicted values. The similar modeling work can be found in Xiong (2013).

#### 2.1.1 Evaluation of Pitzer Binary Interaction Parameters for $\text{Na}^+ - \text{Al}(\text{OH})_4^-$

The equilibrium quotients ( $\log Q_{s4}$ ) for boehmite ( $\text{AlOOH}(\text{cr})$ ) can be expressed as,



$$Q_{s4} = m_{\text{Al}(\text{OH})_4^-} \times m_{\text{H}^+} \quad (2)$$

There are experimental equilibrium quotients ( $\log Q_{s4}$ ) in 0.10-5.0 mol $\cdot$ kg $^{-1}$  NaCl solutions from the literature. In combination of auxiliary data for the  $\text{H}^+ - \text{Cl}^-$  (Holmes et al., 1987) and  $\text{Na}^+ - \text{Cl}^-$  (Pitzer et al., 1984) interactions (Table 1), the equilibrium quotients for Reaction (1) as a function of ionic strength to 250°C are modeled to derive the binary parameters for the  $\text{Na}^+ - \text{Al}(\text{OH})_4^-$  interaction.

**Table 1.** The auxiliary Pitzer binary parameters from the literature used in modeling, and Pitzer parameters derived in this work

Interaction Pairs	Parameter	Temperature Dependence Coefficients*				Original Sources
		a <sub>1</sub>	a <sub>2</sub>	a <sub>3</sub>	a <sub>4</sub>	
H <sup>+</sup> —Cl <sup>-</sup>	β <sup>(0)</sup>	1.77000779E-01	-3.34777082E+01	-2.62214535E-01	1.25778302E-04	Holmes et al., 1987
	β <sup>(1)</sup>	2.92922504E-01	3.40247027E+03	1.97936248E+01	-2.79388381E-02	
	C <sup>ϕ</sup>	3.62000000E-04	-2.91038305E-11	0	-3.03600000E-05	
Na <sup>+</sup> —Cl <sup>-</sup>	β <sup>(0)</sup>	7.45618073E-02	-4.70789056E+02	-1.85114134E+00	1.65564633E-03	Pitzer et al., 1984
	β <sup>(1)</sup>	2.75240690E-01	-5.21117635E+02	-2.88035999E+00	4.71462791E-03	
	C <sup>ϕ</sup>	1.53693372E-03	4.80725476E+01	1.74679979E-01	-1.56268596E-04	
Na <sup>+</sup> —OH <sup>-</sup>	β <sup>(0)</sup>	8.83443913E-02	-1.19784571E+03	-6.10983033E+00	7.43325156E-03	Pabalan and Pitzer, 1987
	β <sup>(1)</sup>	2.44421177E-01	1.62702502E+03	9.48250496E+00	-1.15788697E-02	
	C <sup>ϕ</sup>	3.99943679E-03	8.82475511E+01	4.06876285E-01	-4.75666912E-04	
Na <sup>+</sup> —Al(OH) <sub>4</sub> <sup>-</sup>	β <sup>(0)</sup>	5.1000E-02	0	0	0	This work**
	β <sup>(1)</sup>	2.5324E-04	-2.2335E+04	-1.2278E+02	-1.6695E-01	
	C <sup>ϕ</sup>	-9.0000E-04	3.5669E+01	0	0	
OH <sup>-</sup> —Al(OH) <sub>4</sub> <sup>-</sup>	θ	1.4000E-02	0	0	0	Wesolowski, 1992
Na <sup>+</sup> —OH <sup>-</sup> —Al(OH) <sub>4</sub> <sup>-</sup>	ψ	-4.8000E-03	5.5000E+01	0	0	This work**

\* The temperature dependence expression for Pitzer parameters is

$$x(T) = a_1 + a_2 \times \left( \frac{1}{T} - \frac{1}{298.15} \right) + a_3 \times \ln\left( \frac{T}{298.15} \right) + a_4 \times (T - 298.15)$$

The coefficients for H<sup>+</sup>—Cl<sup>-</sup>, Na<sup>+</sup>—Cl<sup>-</sup>, and Na<sup>+</sup>—OH<sup>-</sup> are from the data0.ypf (Wolery and Jarek, 2003), which were generated by the EXCEL spreadsheet authored by Wijesinghe and Rard (2005).

\*\* The parameters above 25°C are evaluated by this study; the parameters at 25°C are from Wesolowski (1992). Notice that the temperature dependence expression for β<sup>(1)</sup> of Na<sup>+</sup>—Al(OH)<sub>4</sub><sup>-</sup> is fitted by using the values in Table 3, and some accuracy is lost when conforming to the temperature dependence expression.

In modeling the temperature function of binary parameters detailed in Table 1, for Na<sup>+</sup>—Al(OH)<sub>4</sub><sup>-</sup>, β<sup>(0)</sup> is set to a constant value, which is the value at 25°C from Wesolowski (1992). For C<sup>ϕ</sup>, the coefficient, a<sub>2</sub>, for the temperature function expression, is set to 35.669. Then, the equilibrium quotients as functions of temperatures and ionic strengths from Palmer et al. (2001) are modeled for equilibrium constants at infinite dilution, i.e., log K<sub>s4</sub>, and for at β<sup>(1)</sup> at various temperatures. In Table 2, log K<sub>s4</sub> at individual temperatures, and its temperature function expression are tabulated. In Table 3, β<sup>(1)</sup> at individual temperatures are tabulated. Using these individual values for β<sup>(1)</sup>, the coefficients for the temperature function expression are fitted (Table 1).

**Table 2.** Equilibrium constants for Reaction (1) at infinite dilution obtained in this work by using the Pitzer model

T, °C	log $K_{s4}$ , This work	log $K_{s4}$ (Palmer et al., 2001)*
100	-12.89 ± 0.04	-13.02 ± 0.03
150	-12.03 ± 0.05	-12.06 ± 0.03
200	-11.34 ± 0.05	-11.40 ± 0.03
250	-10.98 ± 0.06	-11.05 ± 0.04
Temperature Dependence Expression	$\log K_{s4} = -2526.286 \times \frac{1}{T} - 6.082542$ (T in Kevin)	$\log K_{s4} = -2598.755 \times \frac{1}{T} - 5.991052$ (T in Kevin)

\*The extrapolation to infinite dilution is based on their empirical, weighted fitting equation as functions of ionic strength and temperature.

**Table 3.** Pitzer binary interaction parameters,  $\beta^{(1)}$  and  $C^\phi$  for  $\text{Na}^+ - \text{Al}(\text{OH})_4^-$ , evaluated in this work\*

T, °C	$\beta^{(1)}$	$C^\phi$
100	0.3100	-0.02495
150	0.1971	-0.03624
200	0.5274	-0.04514
250	0.9817	-0.05235

\* Evaluated from equilibrium quotients,  $Q_{s4}$ , in NaCl solutions from Palmer et al. (2001)

### 2.1.2 Evaluation of Pitzer Mixing Interaction Parameters Related to $\text{Al}(\text{OH})_4^-$

In the model developed in this work, the theta parameter,  $\theta_{\text{OH}^-, \text{Al}(\text{OH})_4^-}$ , is set to a constant value of 0.014, which is the value at 25°C from Wesolowski (1992). For the psi parameter,  $\Psi_{\text{Na}^+, \text{OH}^-, \text{Al}(\text{OH})_4^-}$ , its temperature function is modeled from boehmite solubility data in NaOH solutions at 100°C through 130°C from Russell et al. (1955) (Table 4), using the auxiliary data for the  $\text{Na}^+ - \text{OH}^-$  interaction from Pabalan and Pitzer (1987). The reason that solubility data of Russell et al. (1955) are selected for usage in modeling is that they also measured densities of solutions besides solubility. Therefore, their data can be precisely converted to those on molal scale. In addition, their density measurements as functions of base and aluminum concentrations at each temperature can be fitted as the multiple linear regressions, which are useful for conversion of other literature data for the validation test (see the following section). The isothermal multiple linear regressions are tabulated in Table 5.

The temperature dependence function of the psi parameter (Table 1) is constructed based on the values at 100°C through 130°C, and the value at 25°C from Wesolowski (1992). Although the data set from Russell et al. (1955) is from 100°C through 170°C, only those data at 100°C through 130°C are modeled, and the results are used for construction of the mathematical function. The reason for using the results at 100°C through 130°C, in combination with the value at 25°C, to construct the temperature dependence function is that the data from 100°C through 130°C are to higher molalities of NaOH up to ~11 mol•kg<sup>-1</sup>.

Additionally, their data at 140°C through 170°C are not modeled in order to test if the temperature function for the psi parameter can be extended to 170°C, and to build the confidence to extrapolate it to 250°C (Table 1).

In modeling boehmite solubility data in NaOH solutions from Russell et al. (1955), the binary interaction parameters for  $\text{Na}^+ - \text{Al}(\text{OH})_4^-$ , and  $\log K_{s,4}$ , are based on those obtained in the preceding section. With these constraints, the psi parameters as a function of temperature are obtained (Table 4). Based on the psi parameters at individual temperatures, the temperature function of the psi parameters is fitted (Table 1).

**Table 4.** Pitzer ternary interaction parameter,  $\Psi$ , for  $\text{Na}^+ - \text{OH}^- - \text{Al}(\text{OH})_4^-$ , estimated in this work\*

T, °C	$\Psi$
100	-0.04188
110	-0.04572
120	-0.04938
130	-0.05285
140	-0.05615**
150	-0.05929**
160	-0.06229**
170	-0.06516**
180	-0.06790**
190	-0.07052**
200	-0.07303**
210	-0.07543**
220	-0.07774**
230	-0.07996**
240	-0.08209**
250	-0.08414**

\*Estimated from solubility data of boehmite in NaOH solutions from Russell et al. (1955).

\*\*Calculated from the temperature dependence function extrapolated to 250°C.

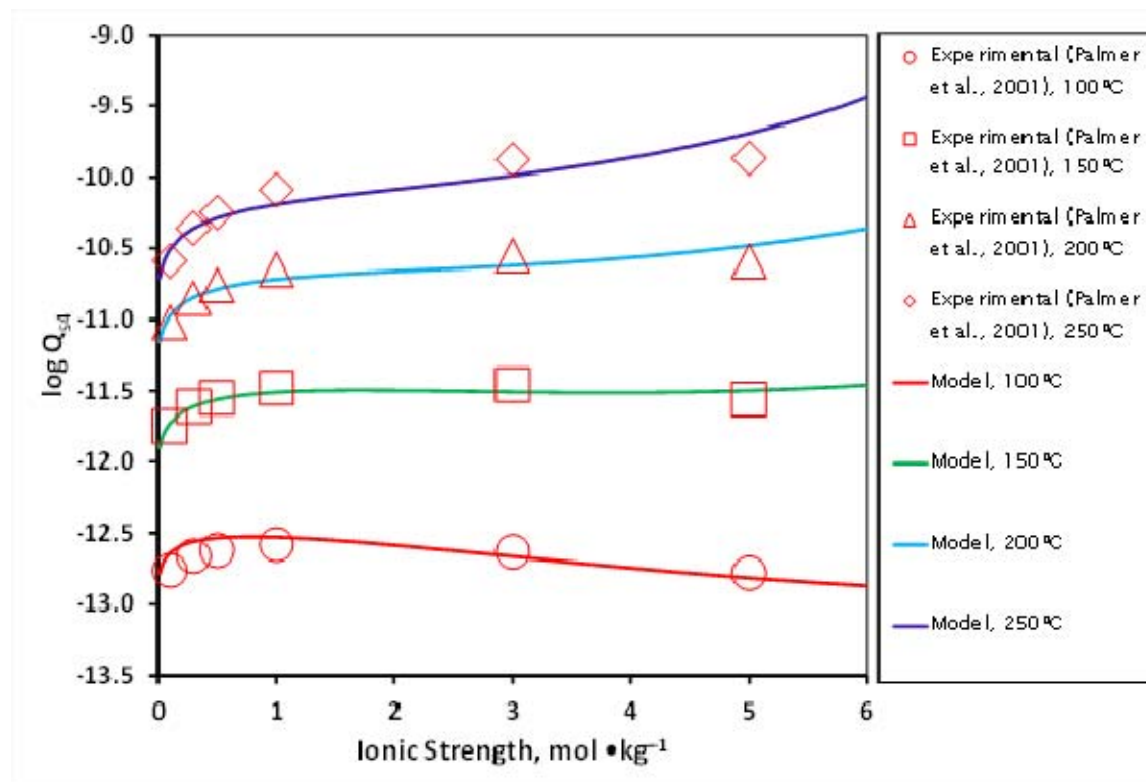
**Table 5.** Multiple linear correlation expressions for density measurements as functions of base and aluminum concentrations\*, based on measurements from Russell et al. (1955)

Temperature, °C	Coefficients		
	a	b	c
100	2.0170E-04	1.5533E-03	0.99909
110	2.9110E-05	1.7219E-03	1.0012
120	-3.3770E-05	1.8330E-03	1.0030
130	4.4992E-04	1.2903E-03	1.0104
140	6.6667E-04	3.0000E-03	0.97267
150	1.6317E-03	-4.1358E-04	1.0309
170	-7.6015E-04	3.1352E-03	0.99437

\* The general correlation expression is:  $\rho \text{ (g/cm}^3\text{)} = a \times C_{\text{Na}_2\text{O}} \text{ (g/L)} + b \times C_{\text{Al}_2\text{O}_3} \text{ (g/L)} + c$

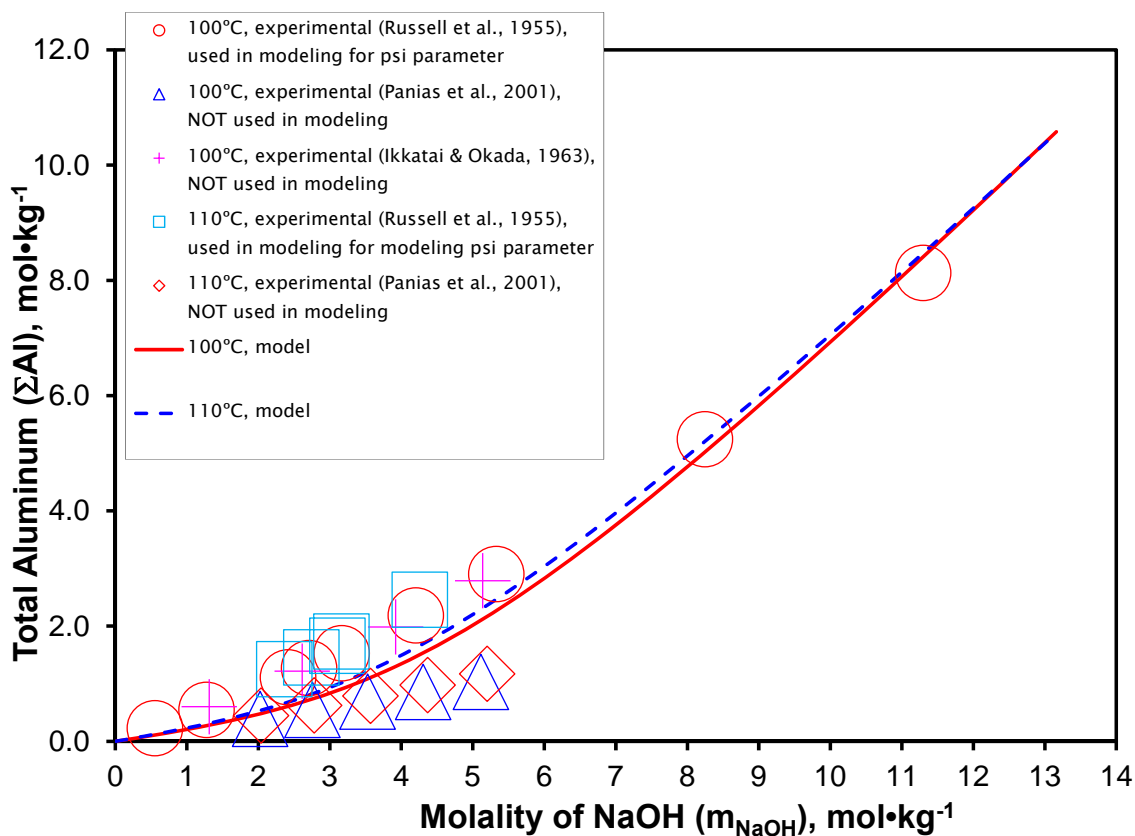
## 2.2 Verification and Validation of the Model Developed in this Work

In Figure 1, the model predicted equilibrium quotients,  $\log Q_{sd}$ , as a function of ionic strength, are compared with experimental values determined by Palmer et al. (2001). Figure 1 demonstrates that the model is excellent in reproducing experimental values.



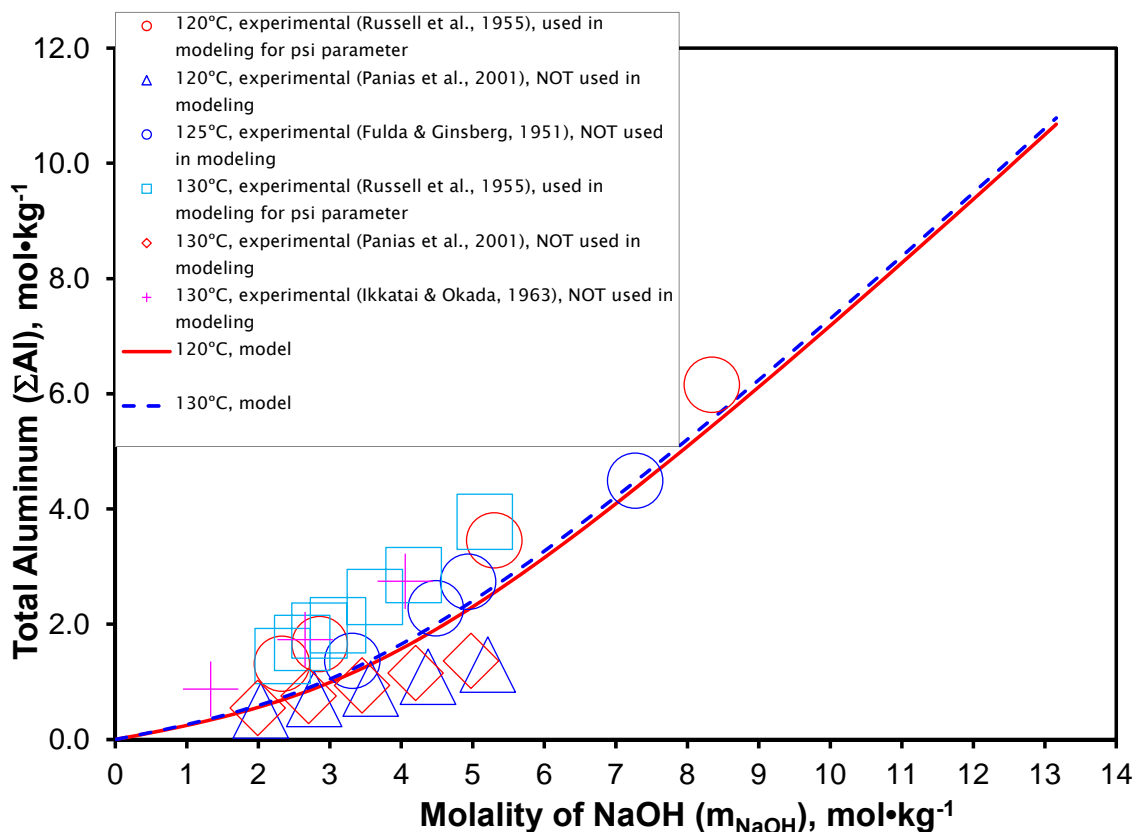
**Figure 1.** A plot showing the model predicted equilibrium quotients as a function of ionic strength in comparison with experimental values. The size of error bars is equal to or smaller than the symbol size.

In Figure 2, solubilities of boehmite as a function of NaOH molality at 100°C and 110°C predicted by the model are compared with experimental values. Notice that experimental data from Ikkatai and Okada (1963) and Panias et al. (2001) are converted to molal scale, based on the densities calculated from the equations in Table 5. This is also true for all other literature data thereafter, if the conversion is necessary. Figure 2 indicates that solubilities predicted by the model are in good agreement with the experimental data from Ikkatai and Okada (1963) and from Panias et al. (2001), which are independent from the model.



**Figure 2.** A plot showing the model predicted solubilities of boehmite at 100 °C and 110 °C as a function of NaOH molality in comparison with experimental values. The size of error bars is equal to or smaller than the symbol size.

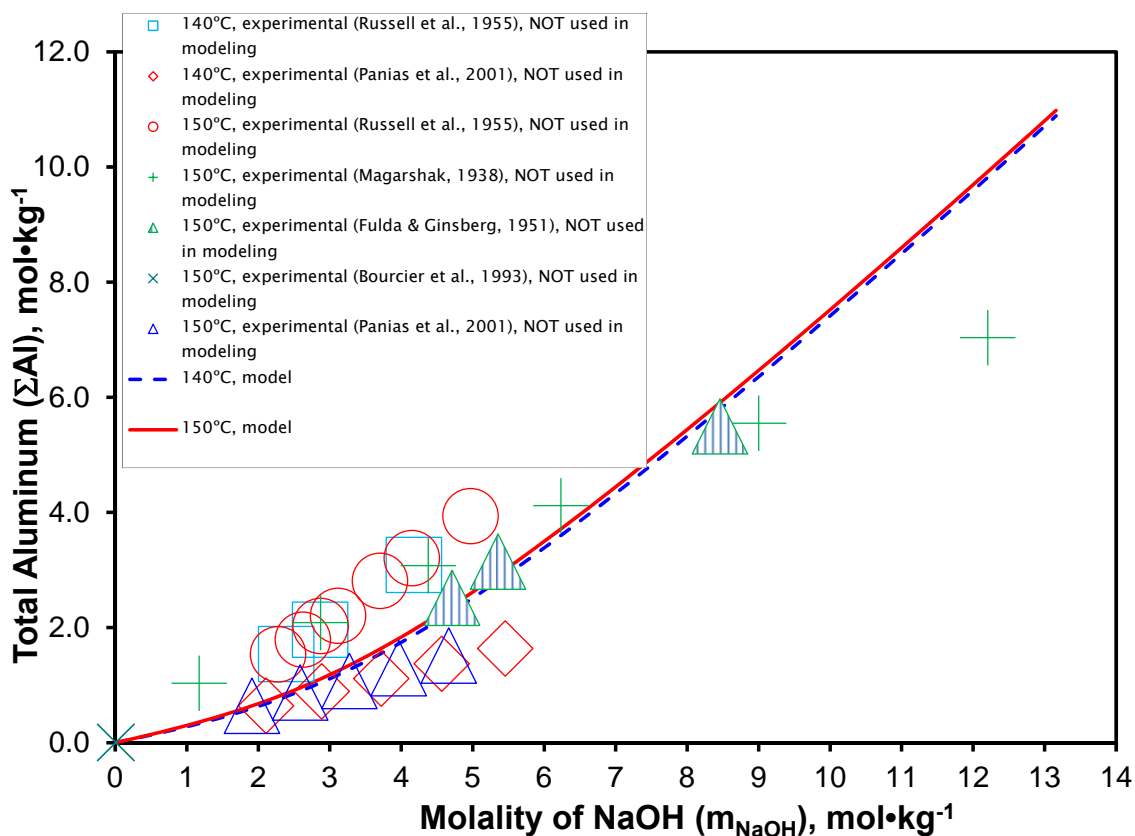
Solubilities of boehmite as a function of NaOH molality at 120°C and 130°C calculated using the model are compared with experimental values (Figure 3). Notice that experimental data from Fulda and Ginsberg (1951) at 125°C, from Ikkatai and Okada (1963) at 130°C, and from Pnias et al. (2001) at 120°C and 130°C are not used in modeling. Figure 3 shows that solubilities predicted by the model are in good agreement with the experimental data independent from the model.



**Figure 3.** A plot showing the model predicted solubilities of boehmite at 120 °C and 130 °C as a function of NaOH molality in comparison with experimental values. The size of error bars is equal to or smaller than the symbol size.

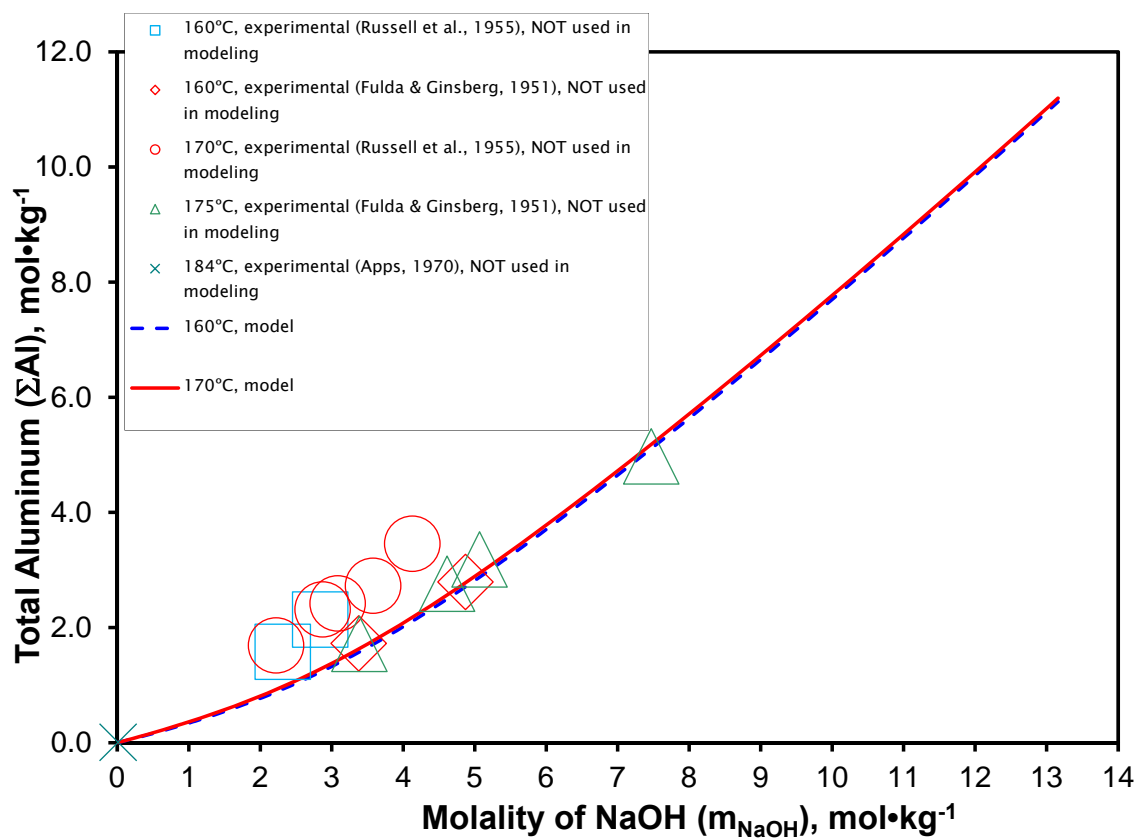
Figure 4 displays solubilities of boehmite as a function of NaOH molality at 140°C and 150°C. It is worth noting that experimental data from Russell et al. (1955), Panias et al. (2001) at 140°C and 150°C, from Magarshak (1938), Fulda and Ginsberg (1952), and Bourcier et al. (1993), all at 150°C, are independent from the model development. Notice that the experiments of Bourcier et al. (1993) were conducted in 0.00186 mol•kg<sup>-1</sup> KOH + 0.0050 mol•kg<sup>-1</sup> B(OH)<sub>3</sub>, and 0.00434 mol•kg<sup>-1</sup> KOH + 0.0050 mol•kg<sup>-1</sup> B(OH)<sub>3</sub> buffer solutions. In the comparison calculations, these two buffer solutions were approximated by 0.00686 and 0.00934 mol•kg<sup>-1</sup> NaOH solutions, respectively. These independent data agree reasonably with the model predicted values, which indicate that the extension of the temperature function of the psi parameter to 150°C is justified.





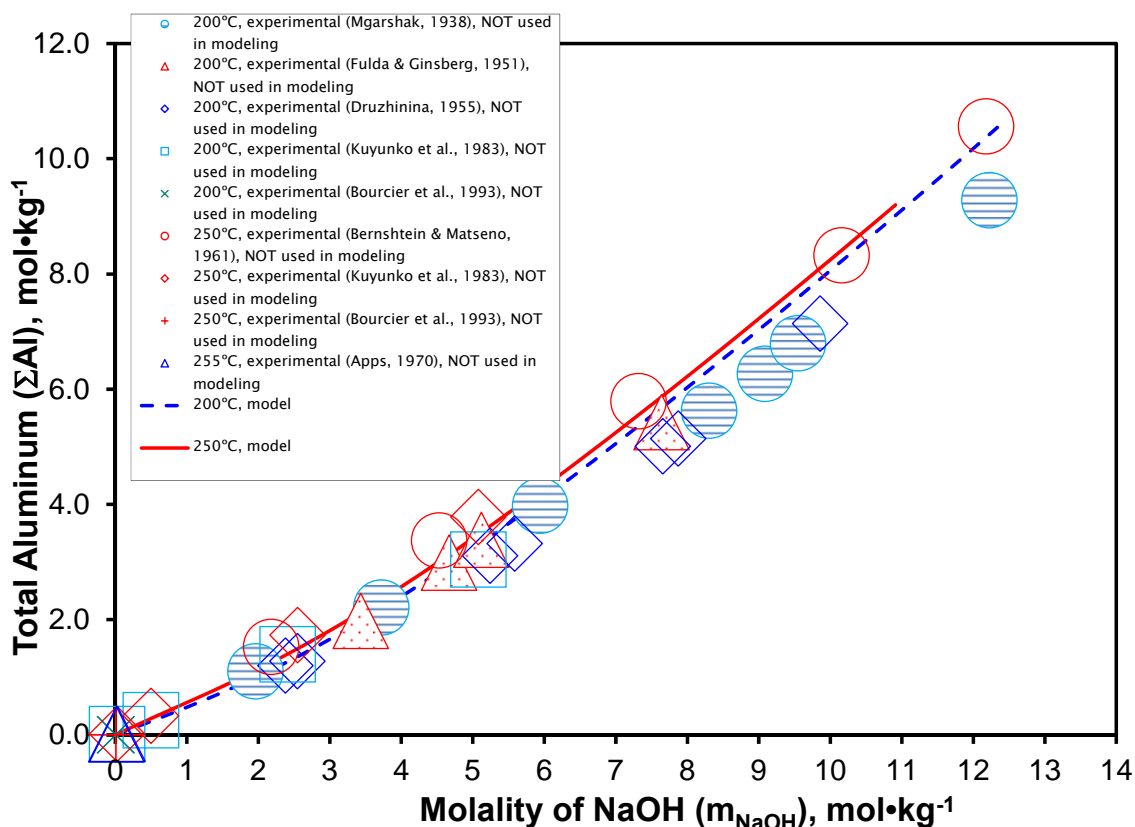
**Figure 4.** A plot showing the model predicted solubilities of boehmite at 140 °C and 150 °C as a function of NaOH molality in comparison with experimental values. The size of error bars is equal to or smaller than the symbol size.

In Figure 5, independent experimental solubility data from Fulda and Ginsberg (1951) at 160°C and 175°C, and from Apps (1970) at 184°C, are compared with the model predicted solubility curves at 160°C and 170°C. Obviously, the model agrees well with the independent experimental data, which provides the confidence in the extension of the temperature function of the psi parameter to 170°C and beyond.



**Figure 5.** A plot showing the model predicted solubilities of boehmite at 160 °C and 170 °C as a function of NaOH molality in comparison with experimental values. The size of error bars is equal to or smaller than the symbol size.

In Figure 6, solubility curves at 200°C and 250°C are constructed by using the model. In the construction, the temperature dependence function for the psi parameter,  $\Psi_{\text{Na}^+, \text{OH}^-, \text{Al}(\text{OH})_4^-}$  estimated based on solubility data of Russell et al. (1955), is extrapolated to 250°C. The independent experimental data from Kuyunko et al. (1983), and Bourcier et al. (1993) at 200°C and 250°C, from Magarshak (1938), Fulda and Ginsberg (1951), Druzhinina (1955), all at 200°C, and from Bernshtein and Matseno (1955) at 250°C, and Apps (1970) at 255°C, are in excellent agreement with the model. Therefore, in addition to other parameters, the temperature dependence function for the psi  $\Psi_{\text{Na}^+, \text{OH}^-, \text{Al}(\text{OH})_4^-}$  is also validated to 250°C.



**Figure 6.** A plot showing the model predicted solubilities of boehmite at 200 °C and 250 °C as a function of NaOH molality in comparison with experimental values. The size of error bars is equal to or smaller than the symbol size.

The parameters related to  $\text{Al(OH)}_4^-$  obtained in this work are of the similar magnitude in respect to the comparable interactions in the literature. For example, regarding 1:1 interaction, the  $\beta^{(1)}$  for  $\text{Na}^+ - \text{OH}^-$  at 25°C and 250°C are 0.2444 and 0.6239, respectively (Pabalan and Pitzer, 1987). In comparison, the  $\beta^{(1)}$  for  $\text{Na}^+ - \text{Al(OH)}_4^-$  at 25°C and 250°C are 0.2500 and 0.9817, respectively (Table 1 and Table 3). The  $\beta^{(0)}$  for  $\text{Na}^+ - \text{OH}^-$  at 25°C and 250°C are 0.07456 and 0.08536, respectively (Pabalan and Pitzer, 1987). The  $\text{Na}^+ - \text{Al(OH)}_4^-$  interaction has a constant value of 0.05100 for  $\beta^{(0)}$  over the temperature range from 25°C to 250°C (Table 1). The  $C^\phi$  values for  $\text{Na}^+ - \text{OH}^-$  at 25°C and 250°C are 0.001537 and -0.004752, respectively (Pabalan and Pitzer, 1987). Similarly, the  $C^\phi$  values for  $\text{Na}^+ - \text{Al(OH)}_4^-$  at 25°C and 250°C are -0.0009000 and -0.05235, respectively (Table 1 and Table 3).

The  $\log K_{sd}$ 's obtained in this study using the Pitzer model are in excellent agreement with those obtained by Palmer et al. (2001) based on the extrapolation to infinite dilution according to their empirical, weighted fitting equation as functions of ionic strength and temperature (Table 2). The  $\log K_{sd}$  at 100°C obtained by this work is  $-12.89 \pm 0.04$  in comparison with their value of  $-13.02 \pm 0.03$  at the same temperature (Table 2). Similarly, the excellent agreement is also observed for the  $\log K_{sd}$ 's at other temperatures (Table 2).

### 3. IMPLEMENTING DOCUMENTS

#### 3.1 Implementing Procedures

This milestone report follows the TP Test Plan for Determining Thermodynamic Properties of Brines, Minerals and Corrosion Products for High Level Radioactive Waste Disposal in Salt (FCRD-UFD-2012-00033) (Xiong et al., 2012) under Task 2.5, *Development of a Chemical Model/database up to 200 °C with High Internal Consistency*.

### 4. TEST EQUIPMENT AND CALIBRATION

This analysis work uses the data from the literature. There is no test equipment or calibration associated with this milestone report.

### 5. RECORDS

This milestone report is developed, maintained, collected, compiled, and submitted in accordance with Sandia National Laboratories records management procedures.

### 6. TRAINING AND QUALIFICATIONS

This analysis work uses the data from the literature. There is no training or qualification associated with this milestone report.

## **7. SOFTWARE**

The aqueous speciation and solubility program EQ3/6 (V. 8.0a) is used for this milestone report.

## **8. PROCUREMENT**

This analysis work uses the data from the literature. There is no procurement associated with this milestone report.

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