IMPORTANT NOTICE: The current official version of this document is available via the Sandia National Laboratories WIPP Online Documents web site. A printed copy of this document may not be the version currently in effect.

Sandia National Laboratories
Waste Isolation Pilot Plant (WIPP)
Test Plan TP 14-02

Experimental Determination of Hydrogen Ion Concentrations in the WIPP Brines without Liquid Junction Potentials

Task 4.4.2.2.1

Rev. 0

Effective Date: March 30, 2015

Prepared by:

Yongliang Xiong (6212)

Sandia National Laboratories
Carlsbad, NM

© 2015 Sandia Corporation
<table>
<thead>
<tr>
<th>Role</th>
<th>Signature Details</th>
<th>Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>Author</td>
<td>Original signed by Yongliang Xiong</td>
<td>March 23, 2015</td>
</tr>
<tr>
<td></td>
<td>Yongliang Xiong (6212)</td>
<td></td>
</tr>
<tr>
<td>Technical Reviewer</td>
<td>Original signed by Shelly R. Nielsen for</td>
<td>3-25-15</td>
</tr>
<tr>
<td></td>
<td>Paul Domski (6212)</td>
<td></td>
</tr>
<tr>
<td>QA Reviewer</td>
<td>Original signed by Shelly R. Nielsen</td>
<td>3-25-15</td>
</tr>
<tr>
<td></td>
<td>Shelly Nielsen (6210)</td>
<td></td>
</tr>
<tr>
<td>Management Reviewer</td>
<td>Original signed by Christi Leigh</td>
<td>3-27-15</td>
</tr>
<tr>
<td></td>
<td>Christi Leigh (6212)</td>
<td></td>
</tr>
</tbody>
</table>
# TABLE OF CONTENTS

1.0 DEFINITION OF ABBREVIATIONS AND ACRONYMS ........................................ 4

2.0 REVISION HISTORY ............................................................................................ 5

3.0 PURPOSE AND SCOPE ...................................................................................... 5

4.0 EXPERIMENTAL PROCESS DESCRIPTION ......................................................... 6
   4.1 Methodology ...................................................................................................... 6
      4.1.1 Experimental Procedure .............................................................................. 9
      4.1.2 Supporting Solutions .................................................................................. 11
   4.2 Sample Control ................................................................................................. 11
   4.3 Data Quality Control ........................................................................................... 11
      4.3.1 Measuring and Test Equipment (M&TE) ...................................................... 11
      4.3.2 Data Acquisition Plan ................................................................................ 11
      4.3.3 Data Identification and Use ....................................................................... 12
   4.4 Equipment ........................................................................................................... 12
      4.4.1 Weighing Equipment ................................................................................... 12
      4.4.2 Liquid Measuring Equipment ................................................................... 12
      4.4.3 Other Analytical Equipment ...................................................................... 12

5.0 TRAINING ............................................................................................................. 13

6.0 HEALTH AND SAFETY ...................................................................................... 14

7.0 PERMITTING/LICENSING .................................................................................. 14

8.0 REFERENCES ....................................................................................................... 14
1.0 DEFINITION OF ABBREVIATIONS AND ACRONYMS

ASTM American Society for Testing and Materials
CBFO US DOE Carlsbad Field Office
CO₂ Carbon dioxide
CRA Compliance Re-Certification Application
DAS Data acquisition system
DOE Department of Energy
EBSD Electron backscatter diffraction
EDS Energy dispersive system
ERDA-6 Energy Research and Development Administration well 6
GC-MS Gas chromatography mass spectrometer
GWB Generic Weep Brine (synthetic Salado Formation brine)
HTPS High temperature potentiometric system
IC Ion chromatograph
ICP-AES Inductively-coupled plasma atomic emission spectrometer
ICP-MS Inductively-coupled plasma mass spectrometer
LANL Los Alamos National Laboratory
M&TE Measuring and test equipment
NIST National Institute of Standards and Technology
NBS National Bureau of Standards
NP Nuclear Waste Management Program Procedure
PA Performance Assessment
SEM Scanning electron microscope
SNL Sandia National Laboratories
SP Activity/Project Specific Procedure
TP Test Plan
TRU Transuranic
WIPP Waste Isolation Pilot Plant
XRD X-ray diffraction
2.0 REVISION HISTORY

This is the original version of this Test Plan (TP).

3.0 PURPOSE AND SCOPE

Accurate determinations of hydrogen ion concentrations, pcH (hydrogen ion concentration on a molar scale), or pmH (hydrogen ion concentration on a molal scale), in the WIPP brines, are important to the geochemical conditions, as hydrogen ion concentrations impact a wide range of issues including actinide solubilities in the WIPP brines. However, measurements of pcH or pmH in the WIPP brines are problematic even at room temperature because the WIPP brines, i.e., GWB and ERDA-6, have respective high ionic strengths of 8.26 m and 5.82 m (Xiong and Lord, 2008), which would produce significant liquid junction potentials when using a glass pH electrode.

In the past, the approach we used to measure the hydrogen ion concentrations of ERDA-6 and GWB at room temperature was to perform Gran titrations by addition of known amounts of H\(^+\) or OH\(^-\) (H\(^+\)\_free, added) into the brines and obtain corresponding readings (H\(^+\)\_observed) with a pH meter. Then, pH readings as the x-axis are plotted against known amounts of H\(^+\) as the y-axis to get the slopes. The logarithm of the slope is then the correction factor that could be used to convert the measured pH readings to hydrogen ion concentrations. However, it has been observed that the linear relationships between H\(^+\)\_free, added and H\(^+\)\_observed are not very good for ERDA-6 and GWB. Numerous titration data points have to be excluded from the linear regressions (Roselle, 2011, and scientific notebooks cited there). Even after exclusion of numerous titration data points, the correction factors are still significantly scattered (Roselle, 2011). For instance, the correction factors for ERDA-6 range from ~0.8 to ~1.2 (Roselle, 2011).

Early in the WIPP program, traditional glass pH electrodes were found to have difficulties in measuring pH at elevated temperatures to 90°C (Krumhansl, 1989). The issue was never resolved because WIPP is a “cold” repository at the ambient temperatures. Now the accurate measurement of hydrogen ion concentrations in the WIPP brines is important to the establishment of pcH or pmH profiles of the WIPP brines as a function of temperature.

The purpose of this test plan is to determine pmH profiles of the WIPP brines as a function of temperature from 25°C to 200°C using the high temperature potentiometric system (HTPS). Specifically, the objectives are as follows,

- Experimental determination of pmH profiles of GWB as a function of temperature.
- Experimental determination of pmH profiles of GWB in equilibrium with the solid assemblage of halite (NaCl)—anhydrite(CaSO\(_4\))—polyhalite(K\(_2\)Ca\(_2\)Mg(SO\(_4\))\(_4\)•2H\(_2\)O) as a function of temperature.
- Experimental determination of pmH profiles of ERDA-6 as a function of temperature.
- Experimental determination of pmH profiles of ERDA-6 in equilibrium with the solid assemblage of halite—anhydrite—polyhalite as a function of temperature.
4.0 EXPERIMENTAL PROCESS DESCRIPTION

4.1 Methodology

As the ionic strengths of GWB and ERDA-6 without any solids (non-equilibrated) are well known, whereas the ionic strengths of GWB and ERDA-6 in equilibrium with the assemblage of halite—anhdrite—polyhalite at elevated temperatures (i.e., equilibrated) are not known, the measurements of their pmH will be dealt with separately. For GWB and ERDA-6 without the solid assemblage, their pmH will be directly measured. For GWB and ERDA-6 with the solid assemblage, their pmH will be determined based on the gibbsite [Al(OH)₃]/boehmite (AlOOH) pmH sensor (Xiong, 2014).

For direct pmH measurements, the HTPS will be calibrated with the reference solutions which have the same ionic strengths as those of GWB and ERDA-6. The reference solutions selected are 2.753 m MgCl₂ (ionic strength, 8.26 m) for GWB, and 1.94 m MgCl₂ (ionic strength 5.82 m) for ERDA-6. In the calibration, the test cell and the reference cell will have the same MgCl₂ solution. Then, known amounts of HCl or NaOH solutions corresponding to at least three pmH values (e.g., pmH 3, pmH 5, pmH 7.5) will be introduced into the test cell to establish the relationships between pmH and electric potential (voltage). After the calibration is performed, the MgCl₂ solution in the test cell will be disposed, the test cell will be washed and cleaned, and either GWB or ERDA-6 will be placed into the test cell. After the electric potential reading is observed, the corresponding pmH value can be obtained, according to the relationship between pmH and electric potential that has been established in the calibration. This can be illustrated in Figure 1.

![Figure 1. An illustration for measuring pmH in GWB](image)

The above straightforward approach cannot be used for measuring pmH in equilibrium with the assemblage of halite—anhdrite—polyhalite at elevated temperatures because the ionic strengths are not known owing to dissolution of these solids as a function of temperatures. The strategy of this work, to measure in situ pmH values in GWB and ERDA-6 in equilibrium with the assemblage of halite—anhdrite—polyhalite at elevated temperatures, is to employ solubility
of gibbsite [Al(OH)$_3$] and boehmite (AlOOH) as pmH sensors (Xiong, 2014). In this approach, the total dissolved concentrations of aluminum on a molal scale ($m_{\Sigma Al}$) directly correspond to pmH as illustrated in Figure 2.

![Figure 2](image)

**Figure 2. An illustration of determination of pmH based on solubility of gibbsite [Al(OH)$_3$] and boehmite (AlOOH) as pmH sensors.**

In the work of Xiong (2014), solubility of boehmite is used as pmH sensor, as Al(OH)$_4^-$ is the dominant species in the pmH range from the slightly acidic to alkaline,

$$\text{AlOOH} (\text{cr, boehmite}) + 2\text{H}_2\text{O} = \text{H}^+ + \text{Al(OH)}_4^- \quad (1)$$

According to Reaction (1), there will be a corresponding concentration of aluminum at the known pmH concentration. Therefore, as soon as the relation between pmH and aluminum concentration is established, the pmH can be determined based on the corresponding aluminum concentration. Figure 3 provides an example from Xiong (2014) for the correlations between pmH (the notation “pH$_m$” in Xiong, 2014) and $m_{\Sigma Al}$ based on solubilities of boehmite in 1.0 and 5.0 m NaCl solutions at 200°C.
Figure 3. An example for the correlations between pmH and $m_{\text{Al}}$ based on solubilities of boehmite in 1.0 and 5.0 mol NaCl solutions at 200°C from Xiong (2014).

Similarly, regarding solubility of gibbsite as pmH sensor, the relevant reaction can be cast as follows,

$$\text{Al} (\text{OH})_3 (\text{cr, gibbsite}) + \text{H}_2\text{O} = \text{H}^+ + \text{Al} (\text{OH})_4^- \quad (2)$$

The gibbsite pmH sensor will be used below 100°C, whereas the boehmite pmH sensor will be used above 100°C (Xiong, 2014). The usage of boehmite as a pmH sensor is well demonstrated by Xiong (2014) in the temperature from 100°C to 250°C. The same principle will be applied to gibbsite in the temperature range from 25°C to 100°C where gibbsite is the stable phase.

Specifically, there are two primary steps that are essential to this work. In the first step, solubilities of gibbsite/boehmite in GWB and ERDA-6 in equilibrium with the assemblage of halite—anhydrite—polyhalite at the known in situ pmH values as a function of temperature will be determined. In situ pmH values will be measured in the HTPS based on acid-base titrations. Then, the relationships between solubilities of gibbsite/boehmite and pmH values can be established based on the results from the first step. In the second step, gibbsite/boehmite will be allowed to be in equilibrium with GWB and ERDA-6 in equilibrium with the assemblage of halite—anhydrite—polyhalite as a function of temperature, without acid-base titrations. According to solubilities of gibbsite/boehmite, the pmH profiles of GWB and ERDA-6 in equilibrium with the assemblage of halite—anhydrite—polyhalite as a function of temperature will be determined based on the relationships established in the first step.
The experiments described in this test plan use the two standard WIPP brines, GWB which represents an idealized brine from the Salado Formation at the repository level, and ERDA-6 brine which represents an idealized composition of brine from Energy Research and Development Administration Well 6 in the Castile Formation, and is the brine which may infiltrate the WIPP repository in the case of human intrusion below the repository. Preparations of GWB and ERDA-6 for this experimental work will follow SP 20-4, Revision 2, *Preparing Synthetic Brines for Geochemical Experiments* (Xiong, 2008). Henceforth, any mention of GWB or ERDA-6 in this test plan will be prepared in accordance with SP 20-4.

4.1.1 Experimental Procedure

**Task 1. Experimental determination of pmH profiles of GWB as a function of temperature**

There are two steps required for the experiments in this task, a calibration step using MgCl₂, and a measurement step to determine the pmH of GWB at elevated temperatures using GWB. In the first step, calibrations will be performed. In the calibration step, 2.753 m MgCl₂ solution will be loaded into the test and reference cells in the HTPS. In the temperature range from 25°C to 200°C at increments of 25°C, known amounts of HCl or NaOH corresponding to at least three pmH values will be introduced into the test cell to establish the relationships between pmH’s and potentials at each temperature.

In the second step, after disposing 2.753 m MgCl₂ solution in the test cell, and washing and cleaning the test cell, GWB will be loaded into the test cell only in the HTPS with 2.753 m MgCl₂ solution still in the reference cell. Potential readings in the temperature range from 25°C to 200°C at increments of 25°C will be acquired. According to the pmH-potential relationships established by the first step of calibration, pmH values of GWB at each temperature will be determined.

**Task 2. Experimental determination of pmH profiles of GWB in equilibrium with the solid assemblage of halite—anhydrite—polyhalite as a function of temperature**

There are two sets of experiments in this task. In the first set of experiments, GWB brine together with the assemblage of halite—anhydrite—polyhalite will be loaded into the test and reference cells in the HTPS. Gibbsite/boehmite will be loaded into the test cell. The pmH-solubility relationships will be established by measuring dissolved Al concentrations in the pmH range from slightly acidic to alkaline, and in the temperature range from 50°C to 200°C at increments of 25°C. Solution samples will be periodically sampled. The sampling schedule depends on the experimental temperature. At lower temperatures, the sampling schedule may be weekly or every fourth day. At higher temperatures, the sampling schedule may be daily or every second day.

In the second set of experiments, GWB brine together with the assemblage of halite—anhydrite—polyhalite, gibbsite or boehmite, will be loaded into the test cell only in the HTPS without the reference cell. The solubilities of gibbsite or boehmite will be determined in the temperature range from 50°C to 200°C at increments of 25°C by measuring the dissolved Al
concentrations. In accordance to the pmH-solubility relationships established by the first set of experiments, pmH values of GWB in equilibrium with the assemblage of halite—anhydrite—polyhalite will be determined. A sampling protocol similar to the first set of experiments in Task 2 will be implemented for these experiments.

Aluminum concentrations will be determined for acidified, diluted samples by using the ICP-AES or ICP-MS. Sodium, potassium, magnesium and calcium concentrations will be determined by using the ICP-AES. Chloride and sulfate concentrations will be determined by the IC. Solid phases will be characterized by using a Bruker XRD with a Sol-X detector.

**Task 3. Experimental determination of pmH profiles of ERDA-6 as a function of temperature**

There are two steps in experiments in this task, a calibration step using MgCl₂, and a measurement step to determine the pmH of ERDA-6 at elevated temperatures using ERDA-6. In the first step, calibrations will be performed. In the calibration step, 1.94 m MgCl₂ solution will be loaded into the test and reference cells in the HTPS. In the temperature range from 25°C to 200°C at increments of 25°C, known amounts of HCl or NaOH corresponding to at least three pmH values will be introduced into the test cell to establish the relationships between pmH’s and potentials at each temperature.

In the second step, after disposing 1.94 m MgCl₂ solution in the test cell, and washing and cleaning the test cell, ERDA-6 will be loaded into the test cell only in the HTPS with 1.94 m MgCl₂ solution still in the reference cell. Potential readings in the temperature range from 25°C to 200°C at increments of 25°C will be acquired. According to the pmH-potential relationships established by the first step of calibration, pmH values of ERDA-6 at each temperature will be determined.

**Task 4. Experimental determination of pmH profiles of ERDA-6 in equilibrium with the solid assemblage of halite—anhydrite—polyhalite as a function of temperature**

There are two sets of experiments in this task. In the first set of experiments, ERDA-6 with the assemblage of halite—anhydrite—polyhalite will be loaded into the test and reference cells in the HTPS. Gibbsite/boehmite will be loaded into the test cell. The pmH-solubility relationships will be established in the pmH range from slightly acidic to alkaline, and in the temperature range from 50°C to 200°C at increments of 25°C.

In the second set of experiments, ERDA-6 with the assemblage of halite—anhydrite—polyhalite will be loaded into the test cell only in the HTPS without the reference cell. Gibbsite/boehmite will be loaded into the test cell. The solubilities of gibbsite/boehmite will be determined in the temperature range from 50°C to 200°C at increments of 25°C. According to the pmH-solubility relationships established by the first set of experiments, pmH values of ERDA-6 in equilibrium with the assemblage of halite—anhydrite—polyhalite at each temperature will be determined.

Aluminum concentrations will be determined for acidified, diluted samples by using the ICP-AES or ICP-MS. Sodium, potassium, magnesium and calcium concentrations will be
determined by using the ICP-AES. Chloride and sulfate concentrations will be determined by the IC. Solid phases will be characterized by using a Bruker XRD with a Sol-X detector.

4.1.2 Supporting Solutions

All supporting solutions will be prepared from reagent grade chemicals from Fisher Scientific or its associated vendors.

4.2 Sample Control

The sample control for the work under this Test Plan will follow WIPP Procedure NP 13-1. Each sample will be appropriately labeled. Sample preparation, utilization, and final disposition will be documented in scientific notebooks. When samples are not in the possession of individuals designated as responsible for their custody, they shall be stored in a secure area with associated documentation (Chain of Custody).

4.3 Data Quality Control

4.3.1 Measuring and Test Equipment (M&TE)

A calibration program will be implemented for the work described in this test plan in accordance with NP 12-1, Control of Measuring and Test Equipment. This M&TE calibration program will meet the requirements in NP 12-1 for: (1) receiving and testing M&TE; (2) technical operating procedures for M&TE; (3) the traceability of standards to nationally recognized standards such as those from the National Institute of Standards and Technology; (4) maintaining calibration records. In addition, NP 13-1 and SP 13-1 identify requirements and appropriate forms for documenting and tracking sample possession. The spreadsheet and other computer based data handling will follow NP 9-1.

4.3.2 Data Acquisition Plan

Data collection procedures are specific to individual instruments. For details of the data acquisition for a particular instrument, see the Specific Procedures (SP) or Users Manual for that instrument. Any data acquired by a data acquisition system (DAS) will be attached directly to the Scientific Notebook or compiled in separate loose leaf binders with identifying labels to allow cross reference to the appropriate Scientific Notebook. If the instrument allows data to be recorded electronically, copies of the data disks will be submitted to the Records Center according to procedure NP 17-1, Records. If possible, data files may be transferred to ZIP disks or CD ROM for submittal to the records center. For instruments that do not have direct data printout, the instrument readings will be recorded directly into the scientific notebook. Current versions of the DAS software will be included in the SNL WIPP Baseline Software List, as appropriate.

The temperature for the furnace for the HTPS will be controlled by the heater panel. The title for the drawing of the heater panel is DWG 13-01-1 “Aqueous High Temperature Heater Controls Heater Panel”.
Quality control of the Scientific Notebooks will be established by procedures described in procedure NP 20-2, *Scientific Notebooks*. Methods for justification, evaluation, approval, and documentation of deviation from test standards and establishment of special prepared test procedures will be documented in the Scientific Notebooks. Procedures including use of replicates, spikes, split samples, control charts, blanks and reagent controls will be determined during the development of experimental techniques.

4.3.3 Data Identification and Use

All calculations performed as part of the activities of TP 14-02 will be documented in a scientific notebook. The notebook will be technically and QA reviewed periodically to ensure that the requirements of procedure NP 20-2, *Scientific Notebooks*, are addressed. If a discrepancy is found, that discrepancy and its resolution will be documented during the review on a Document Review and Comment (DRC) Form NP 6-1-1.

4.4 Equipment

A variety of measuring and analytical equipment will be used for the work described in this test plan. A complete equipment list, including serial numbers, will be maintained in the scientific notebook. Scientific notebooks will be used to record all laboratory work activities.

4.4.1 Weighing Equipment

Several balances are present in the facility and may be used for this project. Balance calibration checks will be performed daily or prior to usage, using the following NBS-traceable weight sets, which, in turn, are calibrated by the SNL Calibration Laboratory. Calibration checks will be recorded in Balance Calibration Records.

4.4.2 Liquid Measuring Equipment

Standard Laboratory Class A glassware (pipettes, volumetric flasks, etc.) will be used at all times. In addition, several adjustable Eppendorf pipettes are available for use in the laboratory. The calibration of pipettes will be checked routinely against a calibrated balance, and will be recorded in the scientific notebook. The accuracy of pipettes will be within ± 1%.

4.4.3 Other Analytical Equipment

- **Ovens and Furnace** - Six Precision Telco Lab ovens are being used to hold samples at elevated temperatures. Temperature is monitored, maintained, and recorded on a daily schedule.
- **pH Meters and Autotitrators** – Solution pH may be measured using pH meters and/or autotitrators. A Mettler Model MA235 pH/Ion Analyzer and a Mettler Model DL25 Autotitrator will be used for this purpose. The range for all pH meters is 0.00 to 14.00. Electrodes will be calibrated before each use or daily (whichever is less
frequent) with a minimum of two pH buffers manufactured by chemical companies with unique lot numbers and expiration dates; traceable to the National Institute of Standards and Technology (NIST). Calibration and calibration checks will be recorded in the scientific notebook.

- **Equipment for Chemical Analysis** – Five instruments may be used for chemical analyses. The first is a Perkin Elmer NexIon 300D Inductively-Coupled Plasma Mass Spectrometer (ICP-MS). The second is a Perkin Elmer Optima 3300 DV Inductively-Coupled Plasma Atomic Emission Spectrometer (ICP-AES); the third is a Cary 300 UV-Visible Spectrophotometer; the fourth, is a UIC, Inc. Carbon Analyzer, consisting of an acidification module, a furnace module, and a CO₂ coulometer, and the fifth is a DIONEX Ion Chromatograph (IC) 3000. These instruments will be user-calibrated per instrument requirement. The ICP-MS and ICP-AES are two primary instruments that will be used.

- **Equipment for Mineralogical, and Textural Characterization** – The mineralogy and texture may be characterized using either an Olympus BX60 Polarizing Microscope or a JEOL JSM 5900LV scanning electron microscope (SEM). Bulk sample mineralogy will be determined using a Bruker AXS D-8 Advance X-Ray Diffractometer (XRD). A mineral standard will be run periodically to verify diffraction line positions.

- **Equipment for Measuring Temperature** – The temperature of the experimental system will be measured with the calibrated thermocouples or the thermocouples verified by the calibrated thermocouples with the data acquisition system (DAS).

- **Equipment for Measuring Voltage** – The voltage of the experimental system will be measured with the voltage meter (Keithley 6517A Electrometer/High Resistance Meter)

The usage of these instruments will follow Activity/Project Specific Procedures (SPs).

### 5.0 TRAINING

All personnel involved in the experiments described in this Test Plan will be trained and qualified for their assigned work. This requirement will be implemented through procedure NP 2-1, *Qualification and Training*. Specifically, the following Nuclear Waste Management Program Procedures (NPs) and Activity/Project Specific Procedures (SPs) are applicable:

- SOP CPG-CHEM-TWD-2011-001 – “ES&H Standard Operating Procedure (ES&H SOP) for Activities in the Sandia National Laboratories/Carlsbad Program Group Laboratory, Building NPHB (U).”
- Standard Operating Procedure (SOP) for Oxygen Deficiency Hazard Alarm Response for Carlsbad (Building NPHB)
- SP 13-1 – “Chain of Custody”
- NP 13-1 – “Control of Samples and Standards”
6.0 HEALTH AND SAFETY

All of the health and safety requirements relevant to the work described in this Test Plan and the procedures that will be used to satisfy these requirements are described in ES&H standard operating procedures. ES&H SOP describes the non-radiological hazards associated with these experiments and describes the procedures to deal with those hazards, including all the training requirements for personnel involved in conducting the experiments. Additional SOPs may be mandated by SNL ES&H requirements and their issuance will not require revision of this Test Plan.

7.0 PERMITTING/LICENSING

There are no special licenses or permit requirements for the work described in this Test Plan.

8.0 REFERENCES


Xiong, Y.-L., 2008. SP 20-4, Preparing Synthetic Brines for Geochemical Experiments, Revision 2. Sandia National Laboratories, Carlsbad, NM.


Xiong, Y.-L., 2014. A Pitzer model for the Na–Al(OH)₄−Cl–OH system and solubility of boehmite (AlOOH) to high ionic strength and to 250 °C. Chemical Geology, 373, 37-49.
This work of authorship was prepared as an account of work sponsored by an agency of the United States Government. Accordingly, the United States Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so for United States Government purposes. Neither Sandia Corporation, the United States Government, nor any agency thereof, nor any of their employees makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately-owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by Sandia Corporation, the United States Government, or any agency thereof. The views and opinions expressed herein do not necessarily state or reflect those of Sandia Corporation, the United States Government or any agency thereof.

Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

Parties are allowed to download copies at no cost for internal use within your organization only provided that any copies made are true and accurate. Copies must include a statement acknowledging Sandia Corporation's authorship of the subject matter.