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Sandia National Laboratories Waste Isolation Pilot Plant (WIPP) Test Plan TP 12-02

Experimental Investigation of Borate Interactions with Rare Earth Elements Under the WIPP Relevant Conditions at Sandia National Laboratories Carlsbad Facility

Task 4.4.2.2.1

Rev. 2

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TABLE OF CONTENTS

1.0	DEFINITION OF ABBREVIATIONS AND ACRONYMS	
2.0	REVISION HISTORY	
3.0	PURPOSE AND SCOPE	
4.0	EXPERIMENTAL PROCESS DESCRIPTION	6
	4.1 Overall Strategy and Process	6
	4.1.1 Experimental Procedure	7
	4.1.2 Supporting Solutions	9
	4.2 Sample Control	9
	4.3 Data Quality Control	9
	4.3.1 Measuring and Test Equipment (M&TE)	9
	4.3.2 Data Acquisition Plan	
	4.3.3 Data Identification and Use	
	4.4 Equipment	
	4.4.1 Weighing Equipment	
	4.4.2 Liquid Measuring Equipment	
	4.4.3 Other Analytical Equipment	
5.0	TRAINING	
6.0	HEALTH AND SAFETY	
7.0	PERMITTING/LICENSING	
8.0	REFERENCES	

1.0 DEFINITION OF ABBREVIATIONS AND ACRONYMS

ASTM	American Society for Testing and Materials
CBFO	US DOE Carlsbad Field Office
CO ₂	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)
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 Procedure
PA	Performance Assessment
SEM	Scanning electron microscope
SNL	Sandia National Laboratories
SP	Activity/Project Specific Procedure
ТР	Test Plan
TRU	Transuranic
WIPP	Waste Isolation Pilot Plant
XRD	X-ray diffraction

2.0 **REVISION HISTORY**

This is the second revision of this Test Plan (TP). In this revision, we include the provision for developing a method for producing overgrowths of new Nd(OH)₃ precipitates on pre-existing crystals (homogeneous nucleation). Because of the very low solubility of Nd(OH)₃ in high pH solutions and the sluggish kinetics of reaction at low temperature, we would like to investigate the kinetics of producing overgrowths first at slightly more acidic conditions (pH = 4 –7). Once we have established this method in these initial experiments, we will then return to higher pH conditions (the conditions of interest to WIPP). In the first revision, the speciation and solubility of Nd(OH)₃ in alkaline regions, and solubility of Nd(OH)₃ at elevated temperatures are to be investigated.

3.0 PURPOSE AND SCOPE

In recent experimental work (Borkowski et al., 2010), it was suggested that the tetraborate ion $(HB_4O_7^-)$ could form a relatively strong complex with trivalent neodymium (Nd(III)), which is one of the rare earth elements and an analog to Am(III). However, the Pitzer interaction parameters regarding the interaction between NdHB₄O₇²⁺ and Cl⁻, and 10-based logarithm of the formation constant (log β_1) of NdHB₄O₇²⁺ itself, have not been validated by independent experimental studies. More importantly, as the WIPP brines (i.e., GWB and ERDA-6) have high concentrations of Na⁺, Mg²⁺, and SO₄²⁻, in order to incorporate the complex AmHB₄O₇²⁺, an analog to NdHB₄O₇²⁺, into the EQ3/6 database to model the contributions of AmHB₄O₇²⁺ to the total soluble Am(III), additional experiments are needed for generation of the required parameters involving Na⁺, Mg²⁺, and SO₄²⁻ as well as validation of parameters produced previously.

The other factor that could also impact the solubility of actinides in geological repositories is the speciation and solubility of actinides in alkaline brines, because the brines that interact with cements in geological repositories could be alkaline. However, the current speciation scheme does not extend to alkaline regions. In addition, the solubility of Nd(OH)₃, a phase that serves as a non-radiologic analog of Am(OH)₃, is not well-constrained, especially under alkaline pH conditions. Because the mobility of actinides will depend upon speciation and solubility, it is desirable to extend the studies of these phenomena into the alkaline region. To achieve the objective of this extension in a timely fashion, we will take advantage of faster reaction kinetics at elevated temperatures, and extrapolate the thermodynamic data back to 25°C with aid of the database "DATA0.YPF".

The purpose of this test plan is to obtain needed Pitzer parameters related to the Nd-borate complex, $NdHB_4O_7^{2^+}$, and to investigate the speciation and $Nd(OH)_3$ solubility in the alkaline region. Specifically, the objectives are as follows,

• Experimental determination of binary interaction parameters (i.e., $\beta^{(0)}$, $\beta^{(1)}$ and C^{ϕ}) for $NdHB_4O_7^{2+}$ — SO_4^{2-} . In GWB and ERDA-6, sulfate concentrations are 0.203 m and 0.187 m, respectively (Xiong and Lord, 2008). Therefore, the interactions between NdHB₄O₇²⁺ and SO₄²⁻ will be important.

- Experimental determination of theta parameters (θ) for NdHB₄O₇²⁺—Na⁺ and NdHB₄O₇²⁺— Mg²⁺. In GWB and ERDA-6, sodium concentrations are 4.04 m and 5.35 m, respectively (Xiong and Lord, 2008). Similarly, magnesium concentrations for GWB and ERDA-6 are 1.16 m and 0.029 m, respectively (Xiong and Lord, 2008). Therefore, the interaction between NdHB₄O₇²⁺ and Na⁺ will be important to predictions of Am(III) solubilities in both GWB and ERDA-6 when the complex of AmHB₄O₇²⁺ is considered. The interaction between NdHB₄O₇²⁺ and Mg²⁺ will be important for GWB.
- Experimental determination of psi parameters (Ψ) for NdHB₄O₇²⁺—Na⁺—CΓ and NdHB₄O₇²⁺—Mg²⁺—CΓ. Psi parameters are important in high ionic strength range. The WIPP brines GWB and ERDA-6 have ionic strengths of 8.26 m and 5.82 m (Xiong and Lord, 2008). In addition to sodium and magnesium concentrations mentioned above, GWB and ERDA-6 have chloride concentrations of 6.40 m and 5.27 m, respectively (Xiong and Lord, 2008). Therefore, these two psi parameters are also needed.
- Experimental determination of speciation of Nd(III) in the alkaline region. Solubility of Nd(OH)₃ as a function of hydroxyl concentrations at various temperatures including elevated temperatures will be investigated. The speciation model obtained will be used for Am(III) as an analog. The solubility data obtained will provide us with key evidence about the thermal function of solubilities of Nd(OH)₃. These data would be compared with the literature data by Wood et al. (2002) and Deberdt et al. (1998) who concluded that the solubilities of rare earth hydroxides, Nd(OH)₃, La(OH)₃ and Gd(OH)₃, are retrograde, meaning that these solids become more insoluble with higher temperature.

4.0 EXPERIMENTAL PROCESS DESCRIPTION

4.1 Overall Strategy and Process

The overall strategy is to use Nd(III) as an analog to actinides in +III state to obtain the needed Pitzer parameters. This is because Nd(III) with coordination number of 6 has an effective radius of 0.983 Å, which is very close to the value of 0.975 Å for Am(III) with the same coordination number (Shannon, 1976), with a difference of 0.82% in radius. In undersaturation experiments, the starting material, Nd(OH)₃, will be purchased if commercially available or synthesized according to the procedure of Wood et al. (2002). Specifically, in order to prepare starting material, Nd(OH)₃, high purity Nd₂O₃ is to react with deionized (DI), deaerated water at 200 °C-250 °C in a Paar® reaction vessel or bolt-closured reaction vessel for two weeks. XRD characterization will be performed to ensure its phase purity after cooling to room temperature, and solid reaction products are dried in nitrogen or argon atmosphere. Dissolved CO₂ will be removed during the deaeration process. The deaeration process will be performed by vigorously bubbling high purity Ar gas through the DI water for at least 30 minutes. Supersaturation experiments will be performed by using dissolved NdCl₃ solutions with Na₂B₄O₇•10H₂O or NaOH.

4.1.1 Experimental Procedure

Task 1. Experimental determination of binary interaction parameters (i.e., $\beta^{(0)}$, $\beta^{(1)}$ and C^{ϕ}) for NdHB₄O₇²⁺—SO₄²⁻.

In the experiments for determination of Pitzer binary interaction parameters for NdHB₄O₇²⁺— SO_4^{2-} , supporting solutions will be a series of Na₂SO₄ solutions with concentrations ranging from 0.01 m to 1.8 m. Solids will be Nd(OH)₃ and Na₂B₄O₇•10H₂O. In the confirmation experiments from supersaturation, the same supporting solutions with Na₂SO₄ will be used. NdCl₃ solutions with initial concentrations of 1.0×10^{-3} m, will be put into Na₂SO₄ solutions. The solid phase will be Na₂B₄O₇•10H₂O. Neodymium concentrations will be determined for diluted samples by using the Perkin Elmer NexIon 300D inductively coupled plasma mass spectroscopy (ICP-MS). Boron concentrations will be measured by using the Perkin Elmer Optima 3300 DV inductively coupled atomic emission spectroscopy (ICP-AES). Hydrogen ion concentrations will be determined by applying the established correction factors in Na₂SO₄ solutions to measured pH readings (Roselle, 2012). Solid phases will be characterized by using a Bruker AXS, Inc., D8 Advance X-ray diffractometer (XRD) with a Sol-X detector.

In this task, experiments are to be conducted from both supersaturation and undersaturation. They will provide the experimental time required to reach equilibrium. This will be the guidance for the experiments in the following tasks, which will be conducted from undersaturation only.

Task 2. Experimental determination of theta parameters (θ) for NdHB₄O₇²⁺—Na⁺ and NdHB₄O₇²⁺—Mg²⁺

In the experiments for determination of the theta parameter (θ) for NdHB₄O₇²⁺—Na⁺, supporting solutions will be a series of NaCl solutions ranging from 0.010 m to 5.0 m. Solids will be Nd(OH)₃ and Na₂B₄O₇•10H₂O. In the experiments for determination of the theta parameter (θ) for NdHB₄O₇²⁺—Mg²⁺, supporting solutions will be a series of MgCl₂ solutions ranging from 0.01 m to 2.0 m. Solids will also be Nd(OH)₃ and Na₂B₄O₇•10H₂O.

Similarly to Task 1, neodymium concentrations will be determined for diluted samples by using the ICP-MS. Boron concentrations will be determined by using the ICP-AES. Hydrogen ion concentrations will be determined by applying the established correction factors in NaCl and MgCl₂ solutions to measured pH readings. Solid phases will be characterized by using a Bruker XRD with a Sol-X detector.

Task 3. Experimental determination of psi parameters (Ψ) for NdHB₄O₇²⁺—Na⁺—C Γ and NdHB₄O₇²⁺—Mg²⁺—C Γ

In the experiments for determination of psi parameters (Ψ) for NdHB₄O₇²⁺—Na⁺—Cl⁻ and NdHB₄O₇²⁺—Mg²⁺—Cl⁻, supporting solutions will be a series of NaCl + MgCl₂ mixtures used previously (Xiong et al., 2010). Solids will be Nd(OH)₃ and Na₂B₄O₇•10H₂O.

Neodymium concentrations will be determined for diluted samples by using the ICP-MS. Boron concentrations will be determined by using the ICP-AES. Hydrogen ion concentrations will be

determined by applying the established correction factors for $NaCl + MgCl_2$ mixtures (Xiong et al., 2010) to measured pH readings. Solid phases will be characterized by using a Bruker XRD with a Sol-X detector.

Task 4. Experimental validation of determined Pitzer parameters concerning $NdHB_4O_7^{2+}$

Synthetic GWB and ERDA-6 brines (Xiong 2008), will be in contact with Mg(OH)₂, Nd(OH)₃, and Na₂B₄O₇•10H₂O. Solution samples will be analyzed for boron, magnesium, and neodymium concentrations using ICP-MS and ICP-AES. The determined Pitzer parameters will be incorporated into the EQ3/6 database. Experimental boron, magnesium, and neodymium concentrations will be compared with the computer predicted concentrations.

Task 5. Experimental determination of speciation of Nd(III) and solubility of $Nd(OH)_3$ in the alkaline region

Solubility experiments with Nd(OH)₃ as a function of hydroxyl concentrations will be conducted at various temperatures including elevated temperatures to take advantage of fast kinetics at elevated temperatures to determine both the speciation of Nd(III) and the solubility of Nd(OH)₃ in the alkaline region. Nd(OH)₃ crystals will be characterized in terms of crystal dimensions using an SEM. If necessary, the Nd(OH)₃ crystals will be segregated by size using standard sieves. The supporting solutions will be a series of NaOH solutions ranging from 0.01 M to 10 M. In order to remove CO₂ that has potentially contaminated or could potentially contaminate NaOH, 0.1 M BaCl₂ will be added into the mother stock solution, i.e., 10 M NaOH, to remove absorbed CO₂, as BaCl₂ can quantitatively remove absorbed CO₂ by precipitation as BaCO₃ (Keener et al., 2001).

Solubility experiments will be carried out in either Teflon/high density polyethylene containers or in our High-TAC system depending on the experimental temperatures. Solubility will be approached from both undersaturated and oversaturated experiments. In undersaturated experiments 0.15 grams of Nd(OH)₃ crystals will be added to solutions at prescribed pH and temperature values. The Nd(OH)₃ will dissolve into the solution until equilibrium conditions prevail. In oversaturated experiments, a similar crystal + solution mixture will be kept at a lower temperature (e.g., room temperature) for a period of time and then heated to the temperature of interest. A low concentration of another rare earth, such as 1.0×10^{-4} m Gd(III)Cl₃ solution, will also be present in the solution, so that when the system is heated to the temperature of interest, overgrowths of $Gd(OH)_3$ will precipitate on the "seed" crystals (Nd(OH)₃) and these overgrowths will contain some Gd. Thus, the presence of overgrowths will be easy to detect using an SEM with EDS or element mapping capabilities. Notice that the solubility in the experiments from the supersaturation might be slightly different from that in the experiments from undersaturation, because the solubility-controlling phase in the supersaturation experiments should be the solid solution of Nd(OH)3 and Gd(OH)3, whereas the solubility-controlling phase in the undersaturation experiments should be the pure end member of Nd(OH)₃.

The first set of experiments will be performed in slightly acidic to neutral pH (4-7) solutions. We will perform initial experiments to work out any potential problems associated with forming overgrowths of newly precipitated Nd(OH)₃ on the partially dissolved cores of the material. The

acetate buffer will be adjusted, possibly with acid and base, to yield a spread of pH values (4-6) and the pH 7 by the HEPES [4-(2-hydroxyethyl)-1-piperazineethanesulfonic acid] 1 mM buffer.

Also note that in order for the elemental mapping with SEM-EDS to be successful, the relatively large crystals of the seed Nd(OH)₃ crystals will be prepared by recrystallization of the synthesized Nd(OH)₃ at elevated temperatures for considerable time.

In the experiments above 100°C, it is difficult to measure the in-situ pH of the solution. In order to constrain the in-situ pH, we will add the mineral boehmite [AlOOH] to the reactor. Boehmite is relatively insoluble, and the concentration of $Al(OH)_4$ in equilibrium with boehmite constrains the pH of the solution (Xiong, 2014).

In the first round of experiments, we will work with dilute solutions until the solubility as a function of temperature and pH are understood. Afterwards, we will begin work with solutions of increasing ionic strength.

The solutions will be sampled at an appropriate frequency (i.e., more often at higher temperatures) and will continue until we are assured that we are at equilibrium. Before sampling, pH measurements for experiments below 100°C will be made with a pH meter that is calibrated at the same temperature for the experiment. For experiments above 100°C, pH will not be measured. After measuring pH for experiments below 100°C, solution samples will be withdrawn from experiments, and immediately filtered using syringe filters and then preserved in acid to await analysis using ICP-MS. At the termination of the experiment, post-run solids will be examined for characterization of morphology and the presence of overgrowths, as appropriate. We will also perform X-ray diffraction on the solids to assure sample purity and crystallinity.

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; and (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.

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 12-02 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. The review will be documented 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 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 $\pm 1\%$.

4.4.3 Other Analytical Equipment

- Ovens and Furnace-Six Precision Telco Lab ovens are being used to hold samples at elevated temperatures, if needed. 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 (SP 12-14). 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 performance 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) (SP 12-31). The second is a Perkin Elmer Optima 3300 DV Inductively-Coupled Plasma Atomic Emission Spectrometer (ICP-AES) (SP 12-9); the third is a Cary 300 UV-Visible Spectrophotometer (SP 12-25); and the fourth is a UIC, Inc. Carbon Analyzer (SP 12-2), consisting of an acidification module, a furnace module, and a CO₂ coulometer, and the fifth is a DIONEX Ion Chromatograph (IC) 3000 (SP 12-22). The current revision for these SPs will be used. 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) (SP 12-17). Bulk sample mineralogy will be determined using a Bruker AXS D-8 Advance X-Ray Diffractometer (XRD) (SP 12-8). A mineral standard will be run periodically to verify diffraction line positions.

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." Evidence of training will be documented through Form NP 2-1-1, "Qualification and Training" and/or Form NP 2-1-2, "Training Record."

Sample preparation procedures, which may vary from sample to sample as work scope evolves, will be detailed in scientific notebooks, in accordance with procedure NP 20-2.

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 Procedure (ES&H SOP) for Activities in the Sandia National Laboratories/Carlsbad Program Group Laboratory, Building NPHB (U)"—SOP CPG-CHEM-TWD-2011-001. 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**

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