LA-UR-25-31841

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Title:	Experimental Strategy to Challenge Actinide Solubility Predictions
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Intended for:	test plan
Issued:	2025-12-04

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LOS ALAMOS NATIONAL LABORATORY
CARLSBAD OPERATIONS

Test Plan, LCO-ACP-26, Revision 1

Experimental Strategy to Challenge Actinide Solubility Predictions

Effective Date: 4-4-22

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ACP-2204-01-05-01

History of Revision

Revision Number	Effective Date	Pages Affected	Description of Revision
0	9/16/21	All	Original Release
1	4-4-22	All	Revised to update the Test Plan and address DOE-CBFO comments received in Brown to Weaver, "Rejection of LANL Carlsbad Test Plan LCO-ACP-26, Revision 0," CBFO:ERCD:MRB:MC:21-0255:UFC 2300.00, dated October 29, 2021."

Table of Contents

1.0 Purpose 4

2.0 Scope 8

3.0 Safety, Quality Assurance, Requirements, References, Acronyms, and Definitions 10

3.1 Safety 10

3.2 Quality Assurance 10

3.3 Requirements 10

3.4 References 13

3.5 Acronyms and Definitions 19

4.0 Responsibilities 20

5.0 Experiment/Task Description 21

5.1 Technical Background 21

5.2 Task 1: Experimental Plans/Approach to Challenge the An(III) WIPP Model 29

5.3 Task 2: Experimental Plans/Approach to Challenge the An(IV) WIPP Model 37

5.4 Task 3: Experimental Plans/Approach to Challenge the An(V) WIPP Model 42

5.5 Task 4: Experimental Plans/Approach to Challenge the An(VI) WIPP Model 49

6.0 Record Requirements 53

6.1 Record Generation and Maintenance 53

7.0 Attachments and Appendices 53

8.0 Training and Qualifications 53

Experimental Strategy to Challenge Actinide Solubility Predictions

1.0 Purpose

The overall purpose of this Test Plan is to describe the experimental strategy and approach that will be used to challenge the Waste Isolation Pilot Plant (WIPP) actinide solubility model. This Test Plan is complemented by two other Test Plans: Test Plan (LCO-ACP-028) centered on re-measuring the oxidation-state-specific colloidal contributions which is still under development and Test Plan LCO-ACP-25 which is titled, "Effects of Radiolysis, Organic Complexation, and Redox Conditions on the Speciation and Oxidation State Distribution of Pu(III/IV)" that evaluates the actinide oxidation-state distribution model for plutonium. The data obtained from the implementation of these Test Plans, when taken together, will help strengthen the scientific basis of the actinide models used in WIPP performance assessment (PA).

The WIPP actinide solubility model is defined by the reactions that describe the predicted speciation and solubility of actinides in the WIPP and are summarized in Appendix SOTERM (US-DOE, 2019, Appendix SOTERM, Section 4). These were initially developed for PA implementation prior to the Compliance Certification Application (CCA) and underwent a major update in 2002 (Giambalvo 2002 a, b, c). This actinide model was strategically designed to be simplistic with a limited number of reactions and was successfully defended in its PA implementation in Compliance Recertification Application (CRA)-2004, CRA-2009, CRA-2014 and CRA-2019. In this sense, it has served the WIPP project very well.

The WIPP actinide solubility model, and correspondingly the mobile concentration model for the actinide source term (see Figure 1), has always been grounded in the understanding that the solubility of actinides is most importantly dependent on their oxidation state. When considering the actinides that contribute to potential release in WIPP PA, there are four oxidation states that are critical in defining this solubility: III, IV, V and VI (see Figure 2 for the WIPP-relevant oxidation states). The solubility model is also coupled with an oxidation state distribution model as well as a colloid model to predict the overall mobile actinide concentrations. These concentrations are what is needed to define the actinide source term used to predict direct brine release (DBR) in the low probability event that brine inundation occurs in the WIPP.

There are a number of reasons why some re-evaluations of the WIPP actinide solubility model is recommended at this time. First, there are newly tabulated formation constants (as Log Ks) and reaction data published by the Nuclear Energy Agency-Thermodynamic Data Base (NEA-TDB) project that may provide an increased scientific defensibility than those currently used in the WIPP database. Second, there are many new data and more importantly new approaches and techniques for redox control and analyses that can be implemented in WIPP-relevant experiments that allow for a more robust experimental approach and strategy for data

collection. Lastly, there were advancements scientifically in the strategic use of analogs, in understanding the high pH speciation of actinides, and an updated WIPP inventory that are not well reflected in the original conceptualization and subsequent 2002 update of the WIPP actinide model.

The main purpose of this Test Plan is to perform a series of screening experiments to identify the needed experiments or, at least, put in place an experimental strategy to challenge the solubility models for each key actinide oxidation state addressed in the WIPP PA. This leads to the following four tasks:

Task 1: Experimental Plans/Approach to Challenge the An(III) WIPP model

Task 2: Experimental Plans/Approach to Challenge the An(IV) WIPP model

Task 3: Experimental Plans/Approach to Challenge the An(V) WIPP model

Task 4: Experimental Plans/Approach to Challenge the An(VI) WIPP model

The achievable timeframe for many of these experiments is to support CRA-2024, but some planned work will extend to CRA-2029 (see individual oxidation-specific discussion of each Task given later).

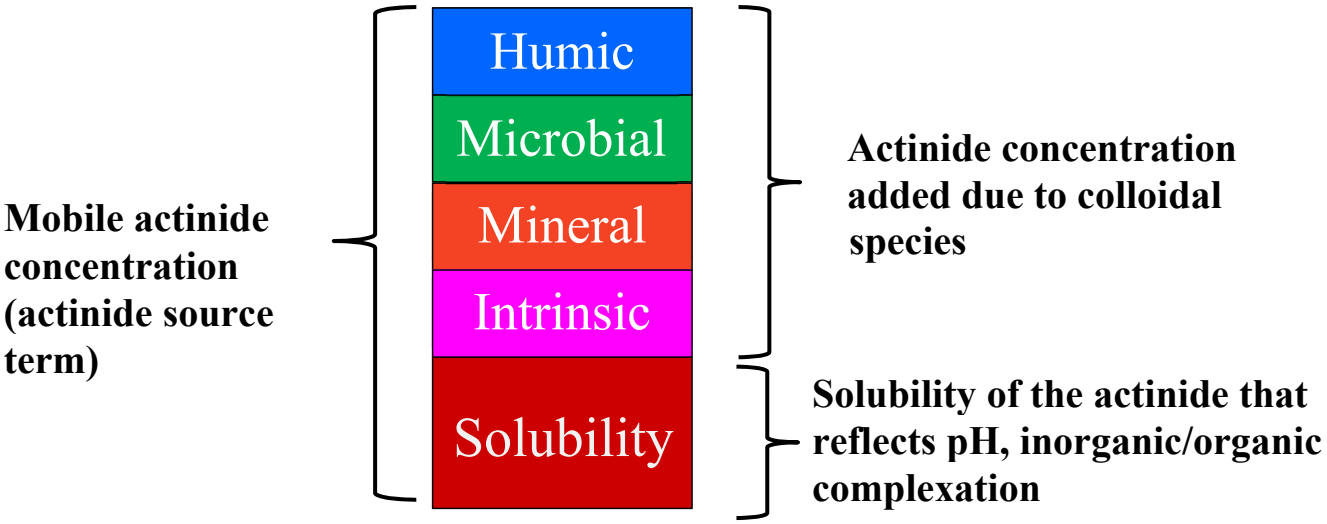


Figure 1. The mobile actinide concentrations used in WIPP PA consists of the sum of all oxidation-state-specific actinide solubilities and the associated colloidal contributions. Four colloidal contributions, humic, intrinsic, mineral and microbial are accounted for in WIPP PA for each oxidation state and actinide.

Most likely actinide oxidation states as a function of Redox

Redox Conditions	Actinide							
	89 Ac	**90 Th**	**91 Pa**	**92 U**	**93 Np**	**94 Pu**	**95 Am**	**96 Cm**
Oxidation States Observed under all Conditions	**3**	(3) **4**	(3) 4 **5**	3 4 5 **6**	3 4 **5** 6 7	3 **4** 5 6 (7)	**3** 4 5 6 7?	**3** 4 5? 6?
⇓								
Oxic Conditions in Groundwater	**3**	**4**	**5**	**6**	**5**	**4** **5**	**3** (5)	**3**
⇓								
Suboxic Zone (mildly reducing)	**3**	**4**	**4**	**4** **6**	**4** *5*	**3** **4**	**3**	**3**
⇓								
Strongly Reducing (e.g., WIPP case)	**3**	**4**	**4**	**4**	**4**	**3** **4**	**3**	**3**

( ) = unstable, ? = claimed but unsubstantiated, **bold** = most stable

Figure 2. The predominance of oxidation states expected in the WIPP repository environment (red enclosed area). For the key multivalent actinides, these are: U(IV), U(VI), Np(IV), Np(V), Pu(III), Pu(IV), Am(III) and Cm(III) (based on Table 33.1 in Reed et al. 2010).

The benefit to the Department of Energy-Carlsbad Field Office (DOE-CBFO) successfully completing the experiments in this Test Plan are:

- For CRA-2024, the four oxidation state models used to calculate actinide solubility in the WIPP will continue to be supported in the following ways:
  - An(III): Data that will improve the description of the solubility controlling phase and organic/borate dependencies will be obtained.
  - An(IV): Data that will confirm the high pH speciation and organic/borate effects will be obtained.

- An(V): Baseline WIPP simulated brine solubilities will be challenged (for the first time), the solubility controlling phase will be confirmed, and organic/borate effects will be evaluated.
- An(VI): Data to challenge the 1 mM U.S. Environmental Protection Agency (EPA) mandated assumption on An(VI) solubility will be obtained. A more realistic upper limit for uranium(VI) solubility may be established. Additionally, some fundamental questions for the incorporation of an An(VI) model will be assessed. Solubility-controlling solids will be identified.

- For CRA-2029, the following additional goals are identified:
  - Data to support a more realistic An(IV) model based on U/Np(IV) as the analog will be obtained.
  - An An(VI) model will be completed.
- Overall, improvements in the An(III) and An(IV) models will permit a more robust assessment of the WIPP actinide oxidation state distribution model (currently a 50/50 split between oxidized and reduced multivalent actinides including plutonium).

2.0 Scope

The scope of this Test Plan is the actinide experimental strategy and scientific investigations needed to challenge/confirm the oxidation-state-specific models in the WIPP actinide solubility model. This will benefit the DOE-CBFO and the WIPP project by strengthening the scientific basis of the actinide solubilities used to calculate the mobile actinide source term used in PA.

There are a number of important aspects to the overall WIPP actinide/brine chemistry model that are outside the scope of this Test Plan. Pitzer parameter analysis and colloidal contributions pertaining to actinides are outside the scope of this Test Plan. The reevaluation of key Pitzer data for some of the underlying brine chemistry is also outside the scope of this Test Plan.

The Los Alamos National Laboratory-Carlsbad Operations (LANL-CO) Actinide Chemistry and Repository Science Program (ACRSP) team will conduct the experiments proposed herein at the Carlsbad Environmental Monitoring Research Center (CEMRC). This Test Plan consists of four tasks, one for each of the key WIPP oxidation states. All tasks will be performed with the lowest activity isotope available to minimize radiolytic effects on the formation constants and/or solubilities measured.

The experimental scope includes but may not be limited to the following:

- Near repository temperature, defined as 23 ± 5 °C.
- WIPP pC_{H+} specific brines (bracketed by Generic Weep Brine [GWB] and U.S. Energy Research and Development Administration [ERDA-6]) as described in procedure ACP-EXP-001 (Brine Preparation). These are generally prepared in 90% formulations (per procedure) to minimize the risk of salt precipitation.
- Simplified brines: $MgCl_2$ and NaCl.
- Presence or absence of carbonate.
- pC_{H+} between 6 and 12.
- Anoxic (N_2) gloveboxes and added redox controls (e.g., Sn or organic reductants) when needed and appropriate.
- The actinides and analogs used for each oxidation state are:
    - An(III) actinides: Pu-242, Am-243, and Nd
    - An(IV) actinides: Th-232, U-238, and Np-237
    - An(V) actinides: Np-237
    - An(VI) actinides: U-238
- The presence and absence of the following organic chelators: Ethylenediaminetetraacetic acid (EDTA), oxalate, citrate and acetate at WIPP-relevant concentrations.
- The presence/absence of borate (when appropriate).

- Ultrafiltration of brine samples using variable pore size (3K, 10K, 30K, 100K) Amicon or Pall ultrafilters. Also ~ 0.22 μm Amicon Ultrafree filters for bulk filtration as needed.
- Aqueous phase analysis of key dissolved species by inductively coupled plasma mass spectrometry (ICP-MS), ion chromatography (IC), ultraviolet- visible-near infrared (UV-Vis-NIR) spectroscopy, and synchrotron-based methods.
- Measurement and/or control of pH (Ross-type electrode) and E_h (Pt electrode).
- Solids analysis by X-ray diffraction (XRD), scanning electron microscopy (SEM), and synchrotron-based methods (X-ray Absorption Near-Edge Structure Spectroscopy [XANES] and Extended X-ray Absorption Fine Structure [EXAFS]).

3.0 Safety, Quality Assurance, Requirements, References, Acronyms, and Definitions

3.1 Safety

The proposed research will be done under the CEMRC safety rules and guidelines according to the current interface agreement between LANL and CEMRC (LCO-ACP-01). The majority of the experimental work proposed in this Test Plan is expected to be done in the actinide chemistry laboratory 151. Some of the low-level work (e.g., U and Th) or non-rad (e.g., Nd) work could also be done in labs 149 or 156 respectively. The actinide experiments proposed that are conducted at CEMRC will be done within the current CEMRC license agreement. LANL project participants, using LANL-CEMRC facilities identified in the relevant safety reviews and statements, will do all the actinide preparations and experiments described herein. In addition to laboratory issues related to the management and use of radioactive materials, this Test Plan encompasses the use of the SEM and XRD equipment currently located in laboratory 152 that will be governed by the safety statements applicable to both instruments.

Low-level radioactive waste generated by the experiments proposed in this Test Plan will be provided to CEMRC for disposal in accordance with the procedures outlined in the LANL-CEMRC interface agreement.

3.2 Quality Assurance

All project participants assigned to work on this Test Plan are responsible for performing work in compliance with the LANL-CO Quality Assurance (QA) Program. The ACRSP Team Leader is responsible to ensure that the technical goals identified in this Test Plan are achieved. The LANL-CO Program Director/Division Leader and ACRSP Team Leader have the overall responsibility for implementation of this Test Plan and compliance with all QA Program requirements.

3.3 Requirements

The data requirements and objectives for the experiments described in this Test Plan are that the data are collected, maintained, and analyzed to Quality Level 1 (QL1) standards (per LCO-QP2-1 and related implementing procedures). Additionally, the following data requirements will be met:

- The data generated must be compatible with the existing WIPP conceptual design as outlined in the 2019-CRA documentation (U.S. DOE, 2019a). Specifically, it is proposed to measure actinide concentrations and or spectra in WIPP-relevant samples to generate Log Ks, ionic strength dependencies and solubilities which are key components of the WIPP PA models used.

- The acceptance criteria for the quality of the data generated, which will consist primarily of the concentration of actinide/analog systems as a function of time, are that the concentrations are known to ± 100% of their actual values. The effects being investigated will lead to three to four orders of magnitude differences in concentration and the WIPP actinide solubilities are typically "order of magnitude" for the PA calculations. The expected uncertainty (both precision and accuracy) in the measurements, specifically ICP-MS analysis, is less than ± 20% which is well within the acceptance criteria needed.
- The representativeness of these data is already established since the primary objective of the proposed experiments is to produce data under the expected WIPP conditions. These data will be directly comparable to other WIPP-relevant data generated previously.
- Although they will be complete as to the stated objective of reproducing data, these data will help define longer-term and more extensive mechanistic work planned for fiscal year 2021 and beyond.
- The following sources of error and uncertainty are identified:
    - Analysis of actinides in WIPP brine, less than 20% for all anticipated concentrations by ICP-MS. Ion chromatography analysis of brine components has an uncertainty of ~10%. Oxidation state uncertainty by XANES is ~10-15%.
    - Redox control and removal of oxygen may be incomplete potentially leading to improper interpretation of the data. The overall uncertainty here is quite low, and therefore negligible, since an anoxic glovebox will be used and the reactivity of the redox controls in these systems will function to complete the oxygen removal process leading to anoxic conditions.
    - Chemical impurities may affect the results. The overall error and uncertainty for this is very low, and therefore negligible, since very high-purity reagents are being used and supporting analyses are being done to confirm the absence of impurities in our system (at least to the level comparable to the initial actinide concentrations).
- There are no data or inputs for the experiments proposed that are beyond the control of the ACRSP.
- All experiments are labeled as specified in the experimental matrix and tracked by this designation throughout in the scientific notebook and associated data packages. Sample tracking, when needed, will be performed according to ACP-IMP-009.
- Data reduction, manipulation, and assessment (including applicable developmental results) will be done according to ACP-IMP-006 and documented in data packages.

The ACRSP program is a well-developed program that relies on implementing and experimental procedures for the full implementation of the Quality Assurance Program Description

requirements. Key Measurement and Test Equipment used in the program, along with the associated uncertainties, are:

Analysis	Technique and Instrument	Uncertainty
Metals/Actinides	ICP-MS (Agilent 7900)	±10% except near limit of detection where it can be as high as ±100%
Organics and Anions	IC (Dionex ICS-6000)	±10% except near limit of detection where it can be as high as ±100%
pH	Ross combination pH electrode	±0.01 (direct measurement) and ± 0.1 for calculated pC_{H+}
E_h	Mettler ORP Pt electrode	± 25 mV
Solids	XRD and SEM	Qualitative characterization of size/composition
Oxidation State (aqueous)	UV-Vis-NIR (CARY 5000 spectrometer)	±1% for most quantitative analyses
Oxidation State (solids)	X-ray Synchrotron (XANES)	±10%

All of these are adequate to achieve sufficient characterization and/or measurement of factors that influence solubility to within ± 20%.

3.4 References

3.4.1 LANL-CO References

LANL-CO Documents

LCO-ACP-01:	LANL-CO/CEMRC Interface Document
LCO-MP7-1:	Procurement
LCO-QP2-1:	Quality Levels and Quality Assurance Requirements
LCO-QP2-3:	Qualification and Training
LCO-QP6-1:	Controlled Document Development, Change, and Revision
LCO-QP17-1:	Record Management
LCO-QPD-04:	LANL-CO Document and Record Management Plan

LANL Reports

LCO-ACP-08:	Actinide (III) Solubility in WIPP Brine: Data Summary and Recommendations
LCO-ACP-09:	Reduction of Higher-Valent Plutonium by Iron Under Waste Isolation Pilot Plant (WIPP)-Relevant Conditions: Data Summary and Recommendations
LCO-ACP-10:	Actinide (VI) Solubility in Carbonate-free WIPP Brine: Data Summary and Recommendations
LCO-ACP-15:	WIPP Actinide-Relevant Brine Chemistry
LCO-ACP-17:	Solubility of An(IV) in WIPP Brine: Thorium Analog Studies in WIPP Simulated Brine
*LCO-ACP-27:	Plutonium Speciation/Solubility in the WIPP

ACRSP Test Plans

LCO-ACP-02:	Solubility/Stability of Uranium (VI) in WIPP Brine
LCO-ACP-03:	Solubility of Neodymium (III) in WIPP Brine
LCO-ACP-04:	Plutonium (VI) Reduction by Iron: Limited-Scope Confirmatory Study
LCO-ACP-05:	Plutonium Speciation and Solubility in the WIPP
LCO-ACP-06:	Americium Solubility/Stability in WIPP Brine
LCO-ACP-07:	Effect of Acetate, Citrate, EDTA, Oxalate and Borate Ions on Neodymium solubility in WIPP Brine
LCO-ACP-25:	Effects of Radiolysis, Organic Complexation, and Redox Conditions on the Speciation and Oxidation State Distribution of Pu(III/IV)
*LCO-ACP-28:	Actinide Colloid Parameters under WIPP-Relevant Conditions

ACRSP-Specific Documents and Procedures

ACP-EXP-001: Brine Preparation
ACP-EXP-002: pH Electrode/Meter Calibration
ACP-EXP-003: Balance Performance Check
ACP-EXP-004: Pipet Performance Checks
ACP-EXP-005: Thermometer Calibration and Performance Check
ACP-EXP-006: UV-Vis-NIR Spectrophotometer Calibration and Performance Check
ACP-EXP-010: Determination of Hydrogen Ion Concentration in Brine
ACP-EXP-011: Inductively Coupled Plasma-Mass Spectrometry
*ACP-EXP-013: Synthesis of Oxidation State Pure Actinide Standards
*ACP-EXP-015: Scanning Electron Microscopy Analysis of Solid Phases
*ACP-EXP-017: X-ray Absorption Spectroscopy of ACRSP Samples
ACP-IMP-002: ACRSP Duplicate File and Working Documents
ACP-IMP-003: Test Plan and Task Implementation Plan
ACP-IMP-004: Measuring and Test Equipment
ACP-IMP-005: Scientific Notebooks
ACP-IMP-006: Data Packages
ACP-IMP-007: Scientific Investigations
ACP-IMP-009: Sample Tracking

**Procedures, Test Plans and reports under development.*

3.4.2 Literature References

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3.5 Acronyms and Definitions

ACRSP:	Actinide Chemistry and Repository Science Program
ASTP:	WIPP Actinide Source Term Program (~ 1990's research)
An:	Generic Actinide
Br^-:	Bromide anion
CCA:	Compliance Certification Application
CEMRC:	Carlsbad Environmental Monitoring Research Center
CFR:	Code of Federal Regulations
CH:	Contact Handled
Cl^-:	Chloride anion
CRA:	Compliance Recertification Application
DBR:	Direct Brine Release
DOE-CBFO:	(U.S.) Department of Energy, Carlsbad Field Office
EDTA:	Ethylenediaminetetraacetic Acid
EPA:	(U.S.) Environmental Protection Agency
ERDA-6:	(U.S.) Energy Research and Development Administration (WIPP well) 6, a synthetic brine representative of fluids in the Castile brine reservoirs
EXAFS:	Extended X-ray absorption fine structure
Fe:	Iron with an unspecified oxidation state
GWB:	Generic Weep Brine, a synthetic brine representative of intergranular Salado-Formation brines
H_2:	Hydrogen
H_2O:	Water
I:	Ionic strength
IC:	ion chromatography
ICP-MS:	Inductively Coupled Plasma, Mass Spectrometry
LANL-CO:	Los Alamos National Laboratory-Carlsbad Operations
Log (K)	Logarithm (base 10) of the formation constant for a complex
M:	molarity, moles of solute per liter of solvent
m:	molality, moles per Kg of solvent
Na^+:	Sodium cation
NEA:	Nuclear Energy Agency
NEA-TDB:	Nuclear Energy Agency-Thermodynamic Data Base
NMR:	Nuclear Magnetic Resonance
$OH^{\cdot}$:	Hydroxyl free radical
PA:	Performance Assessment
PABC:	Performance Assessment Baseline Calculation
PAIR:	Performance Assessment Inventory Report
PAVT:	Performance Assessment Verification Test
Pu:	Plutonium with an unspecified oxidation state

Pu^{3+}: Plutonium in the +3 oxidation state, also written Pu(III)
Pu^{4+}: Plutonium in the +4 oxidation state, also written Pu(IV)
PuO_2: Plutonium (IV) oxide solid
PuO_2^{+}: Aqueous form of the plutonium ion in the V oxidation state, plutonyl
PuO_2^{2+}: Aqueous form of the plutonium ion in the VI oxidation state, plutonyl
QA: Quality Assurance
QL1: Quality Level 1
RH: Remote Handled
SEM: Scanning Electron Microscopy
SNL: Sandia National Laboratories
SOTERM: Actinide source term appendix to support WIPP PA
THEREDA: Thermodynamic Reference Data Base
TIP: Task Implementation Plan
TRU: Transuranic
UV-Vis-NIR: Ultraviolet-visible-near infrared spectroscopy
XANES: X-ray absorption near-edge structure spectroscopy
XRD: X-ray diffraction
WDS: Waste Data System
WIPP: Waste Isolation Pilot Plant

4.0 Responsibilities

Not Applicable.

5.0 Experiment/Task Description

The technical background and general description of the four tasks in this scientific investigation are given in this section. Detailed descriptions of the technical approach and experimental matrices will be either summarized in this Test Plan, documented in the scientific notebooks, or developed later (if needed) as Task Implementation Plans (TIPs) according to procedure ACP-IMP-003.

5.1 Technical Background

5.1.1 Waste Isolation Pilot Plant

The WIPP is located in the northern portion of the Delaware Basin in southeastern New Mexico east of Carlsbad. It was certified by the EPA in May 1998 as a Transuranic (TRU) waste repository and it is currently operated by the DOE-CBFO. The regulatory guidelines for the WIPP are given in 40 Code of Federal Regulations (CFR) 191/194 (U.S. DOE 1996). Based on these regulations, the WIPP is required to undergo re-certification by the EPA every five years. The WIPP was recertified in 2004 (U.S. DOE 2004), 2009 (U.S. DOE 2009), 2014 (U.S. DOE 2014) and CRA-2019 (U.S. DOE 2019a) was submitted and is currently under review by the EPA.

In this regulatory context, the primary goal of the ACRSP experimental program at the CEMRC facility is to support these ongoing WIPP re-certifications and, correspondingly, the associated PA activities. The overall emphasis in this program is on the environmental chemistry of actinides under the conditions expected in the repository. These data/results are used to improve, assess and strengthen the scientific basis for the WIPP repository license.

5.1.2 WIPP Actinide Source Term

The WIPP actinide source term is defined as the sum of the mobile actinide concentrations for the actinides that contribute to potential WIPP release. This consists of the actinide solubilities and the associated estimates of colloidal species that also may be present. The most comprehensive description of the basis for the source term currently used in PA can be found in CRA-2019, Appendix SOTERM (U.S. DOE 2019b).

Historically, the actinide solubility model, which is the focus of this Test Plan, was developed prior to the initial WIPP license application. A significant amount of this research was performed during the 1990s as part of the WIPP Actinide Source Term Program (ASTP) managed by Sandia National Laboratories (SNL) to support the certification of the WIPP. The actinide solubilities calculated based on data available (Trovato 1997; Brush and Xiong 2003; Hobart and Moore 1996) during this time are summarized in Table 1. The goal of the ASTP was to determine the amount of actinides present in WIPP disposal rooms that could be mobilized by contact with brine and possibly migrate from the WIPP to the accessible environment. It featured the development of a numerical model based on the Pitzer approach for high ionic

strength systems to predict mobile actinide concentrations with order-of-magnitude accuracy. This accuracy requirement reflected the expected precision in the PA calculation for EPA compliance (Novak 1995).

Table 1. Actinide Solubilities (M) Calculated (+III, +IV, and +V) or Estimated (+VI) for the CRA-2004 PA, the 1997 PAVT and the CCA PA (Table SOTERM-2, U.S. DOE 2004). The CRA calculations reflect the inclusion of organic complexation and updated chemical conditions for microbial and non-microbial vectors.

Actinide Oxidation State, and Brine	CRA Solubilities, Microbial Vectors	CRA Solubilities, Non-microbial Vectors	PAVT Solubilities	CCA Solubilities
+III, Salado brine	3.07×10^{-7}	3.07×10^{-7}	1.2×10^{-7}	5.82×10^{-7}
+III, Castile brine	1.69×10^{-7}	1.77×10^{-7}	1.3×10^{-8}	1.3×10^{-8}
+IV, Salado brine	1.19×10^{-8}	1.24×10^{-8}	1.3×10^{-8}	4.4×10^{-6}
+IV, Castile brine	2.47×10^{-8}	5.84×10^{-9}	4.1×10^{-9}	6.0×10^{-9}
+V, Salado brine	1.02×10^{-6}	9.72×10^{-7}	2.4×10^{-7}	2.3×10^{-6}
+V, Castile brine	5.08×10^{-6}	2.13×10^{-5}	4.8×10^{-5}	2.2×10^{-6}
+VI, Salado brine	8.7×10^{-6}	8.7×10^{-6}	8.7×10^{-6}	8.7×10^{-6}
+VI, Castile brine	8.8×10^{-6}	8.8×10^{-6}	8.8×10^{-6}	8.8×10^{-6}

The laboratory data for the ASTP were collected at Florida State University, Pacific Northwest Laboratory, Argonne National Laboratory, and Los Alamos National Laboratory. Experimental methods included potentiometric titration, extraction, spectroscopic methods, and solubility experiments. More specifically, solubility data for the An(III) and An(IV) oxidation states were measured at Pacific Northwest National Laboratory (Rai et al. 1995; Rai et al. 1997; Rai et al. 1998). Data for the solubility of the An(V) oxidation state was collected at Lawrence Berkeley National Laboratory and Los Alamos National Laboratory (Runde 2000). Data for the solubility of the An(VI) oxidation state were obtained at Lawrence Livermore National Laboratory (Allen et al. 1997). The effects of organic ligands on dissolved actinide concentrations were evaluated at Florida State University (Choppin et al. 2001). Lastly, a test of the predictive ability of the actinide solubility model was performed at Argonne National Laboratory (Reed et al. 1998; Reed et al. 2003).

In 2002, as briefly discussed earlier, there was a major update to the actinide model used in the CCA (Giambalvo 2002 a, b, c). This model, with relatively few changes in the actinide

reactions, Log Ks and Pitzer parameter, has been implemented for each of the subsequent CRAs. This model was last implemented in the CRA-2019 documentation and the currently calculated actinide solubilities are shown in Table 2. Since CRA-2004, the U(VI) solubility was fixed by the EPA at 1 mM and is the only An(VI) actinide considered in PA. For this reason, there is no An(VI) model and no solubility data are shown for this oxidation state.

Table 2. Historical Actinide Solubilities Calculated for the CRA-2004 PABC, the CRA-2009 PABC, CRA-2014 PA (Brush and Domski 2013, Table SOTERM-13), and CRA-2019 (Domski and Sisk-Scott 2019). (Based on Table 30, CRA-2019 Appendix SOTERM).

Actinide Oxidation State, and Brine	CRA-2004 PABC (M)	CRA-2009 PABC (M)	CRA-2014 PA (M)	CRA-2019 PA (M)
III, GWB	3.87×10^{-7}	1.66×10^{-6}	2.59×10^{-6}	1.63×10^{-7}
III, ERDA-6	2.88×10^{-7}	1.51×10^{-6}	1.48×10^{-6}	1.78×10^{-7}
IV, GWB	5.64×10^{-8}	5.63×10^{-8}	6.05×10^{-8}	5.45×10^{-8}
IV, ERDA-6	6.79×10^{-8}	6.98×10^{-8}	7.02×10^{-8}	5.44×10^{-8}
V, GWB	3.55×10^{-7}	3.90×10^{-7}	2.77×10^{-7}	4.02×10^{-7}
V, ERDA-6	8.24×10^{-7}	8.75×10^{-7}	8.76×10^{-7}	1.20×10^{-6}
VI, GWB/ ERDA-6*	1.00×10^{-3}	1.00×10^{-3}	1.00×10^{-3}	1.00×10^{-3}
*An(VI) solubility is fixed to be 0.001 M by EPA directions (U.S. EPA 2005).				

5.1.3 CRA-2019 Brine Composition, Actinide Inventory, and Emplaced Materials Inventory

The projected inventory (actinides, emplaced materials and organics present) in the WIPP is an important contributor to the approach used to evaluate the relative importance and experimental design to measure actinide solubilities. These inventories were summarized in CRA-2019 Appendix SOTERM and are reproduced here to make the Test Plan somewhat self-standing.

The predicted range in brine composition expected in the WIPP is shown in Table 3. In the WIPP, high ionic strength brines will form when the intruded brine reacts with the emplaced

materials. These brines are Na/Mg/Cl dominated with lesser amount of calcium, borate, sulfate, potassium, lithium, bromide, and carbonate.

The emplaced materials contribute to many aspects of the WIPP repository chemistry that needs to be evaluated. The MgO engineered barrier helps buffer the pH at ~ 9, the iron and other reduced metals are key to establishing the redox environment, and the organics that are potentially present in WIPP complex the actinides and often define the key/major actinide solution chemistry. These inventory data are summarized in Table 4. Most importantly, there is enough MgO added to fully buffer the pH and sequester excess carbonate should this be generated by microbial processes. Additionally, there is excess reduced iron in the WIPP repository and the reactivity associated with this iron is critical in defining the highly reducing conditions expected.

Table 3. WIPP-relevant Brine Compositions as a Function of pC_{H+}. Data are based on the Experimental GWB (100% Saturated Formulation) pH Titration Experiments. Composition of Full-strength GWB and ERDA-6 Brines (100% Saturated Formulation) is also given (Table CRA-2019 SOTERM -5).

pC_{H+}	Element/Species - Measured Concentrations (M)								
	Na^+	K^+	Mg^{2+}	Ca^{2+}	Li^+	$B_4O_7^{2-}$	Cl^-	SO_4^{2-}	Br^-
GWB	3.53	0.467	1.02	1.38×10^{-2}	4.48×10^{-3}	3.95×10^{-2}	5.60	0.177	2.66×10^{-2}
9	3.50	0.458	1.03	1.35×10^{-2}	3.75×10^{-3}	3.89×10^{-2}	5.43	0.176	2.35×10^{-2}
9.5	3.72	0.459	0.850	1.31×10^{-2}	3.70E-03	1.64×10^{-2}	5.55	0.176	2.42×10^{-2}
10	4.59	0.450	0.117	1.34×10^{-2}	3.57×10^{-3}	2.77×10^{-3}	5.35	0.169	2.34×10^{-2}
10.5	4.91	0.454	2.86×10^{-2}	1.24×10^{-2}	3.54×10^{-3}	1.66×10^{-2}	5.39	0.169	2.32×10^{-2}
ERDA-6	4.87	0.0970	1.90×10^{-2}	1.20×10^{-2}	N/A	1.58×10^{-2}	4.80	0.170	1.10×10^{-2}
11	4.96	0.449	0.111	1.09×10^{-2}	3.54×10^{-3}	3.05×10^{-2}	5.31	0.168	2.30×10^{-2}
12	5.02	0.454	0.105	6.97×10^{-3}	3.46×10^{-3}	3.29×10^{-2}	5.31	0.169	2.32×10^{-2}
13	5.11	0.452	9.74×10^{-3}	2.14×10^{-3}	3.55×10^{-3}	2.99×10^{-2}	5.32	0.167	2.35×10^{-2}

N/A – not applicable

The organic inventories are also important as they, in many cases, define the predominant aqueous speciation predicted. These inventories change significantly in each CRA cycle. The CRA-2019 projected inventories lead to the concentrations shown in Table 5. These

concentrations are the maximum ones predicted and bound the range in organic concentrations evaluated experimentally.

Lastly, the actinide inventory is given in Table 6. Plutonium, which is the most important TRU component, will always be present in excess during the WIPP 10,000 year operational period. Americium and curium are essentially inventory limited (always true for Cm, for Am this is true after 5000 y only if sorption is ignored) and are mostly solubilized once brine inundation occurs and decay significantly during the 10,000 year timeframe. In this sense, they are potentially important early in repository history but not over the duration of the operational period. Thorium and uranium are present in enough quantities to remain solubility limited throughout repository lifetime. Neptunium inventories were historically too low for consideration and this oxidation state was largely ignored in past CRAs. This is no longer true and a more comprehensive experimental challenge of these currently predicted An(V) solubility in the WIPP is a major goal of this Test Plan. The ratio of the inventory to the projected solubility is shown in Table 7. These quantify what was just stated regarding the inventory limitation of the key contributors to actinide release in PA.

Table 4. Total Projected Inorganic Waste, Packaging and Emplacement Materials in the WIPP Repository (PAIR 2012 and PAIR 2018). (Based on CRA-2019, Table SOTERM-3).

Material	Source/Type	CRA-2014[1] (Data Cutoff: December 31, 2011)		CRA-2019[2] (Data Cutoff: December 31, 2017)	
		Amount by component or source (kg)	Total (kg)	Amount by component or source (kg)	Total (kg)
Aluminum-based Metals/Alloys	CH and RH Waste	N/A	4.57×10^5	N/A	5.56×10^5
Lead	Packaging	N/A	8.28×10^3	N/A	1.38×10^7
Iron-based Metals/Alloys	CH and RH Waste	N/A	1.22×10^7	N/A	1.54×10^7
Other Inorganic Materials	CH and RH Waste	N/A	7.37×10^6	N/A	1.05×10^7
Other Metal/Alloys	CH and RH Waste	N/A	1.23×10^6	N/A	9.83×10^5
Cement[3]	Reacted	4.22×10^6	1.08×10^7	2.33×10^6	8.88×10^6
	Unreacted	0		3.20×10^3	
	Combination	6.55×10^6		6.55×10^6	
Soils	CH and RH Waste	N/A	5.94×10^6	N/A	5.01×10^6
MgO	Emplacement	N/A	51,430 tons	N/A	>51 tons

[1] PAIR-2012 (Van Soest 2012)
[2] PAIR-2018 (Van Soest 2018)
[3] Contains only site reported data since not specifically tracked in the Waste Data System (WDS) – reacted means already fully hydrated, combination means that a combination of reacted and unreacted cement was reported.
N/A – Not Applicable

Table 5. Range in Concentration of Acetate, Oxalate, Citrate and EDTA in the WIPP Repository Should Brine Inundation Occur (Domski et al. 2019). These are Calculated Based on the Project Inventory and the Minimum Brine Volume (17,400 m^3) for DBR (Table CRA-2019 SOTERM-6).

Organic Complexant	*Concentration at 1X dilution (M)	*Concentration at 5 X dilution (M)	Potential Impact on Actinide Solubility
Acetate	2.83×10^{-2}	5.67×10^{-3}	Relatively low. Weak complexant and highly biodegradable.
Oxalate	1.13×10^{-2}	2.26×10^{-3}	Relatively low. Weak complexant and highly biodegradable.
Citrate	2.30×10^{-3}	4.61×10^{-4}	Moderate. Strong complexant, but likely degraded under WIPP conditions.
EDTA	7.92×10^{-5}	1.58×10^{-5}	High. Very strong complexation. Likely recalcitrant under WIPP conditions.

*1X and 5X refer to the dilution factor relative to the minimum brine volume needed for DBR.

Table 6. CRA-2019 WIPP Radionuclide Inventory Decay-Corrected to 2033 (Table CRA-2019 SOTERM -11).

Selected Radionuclides	Activity (Ci)	Amount (kg)	Element-Specific Inventory (all reported isotopes)	CRA-2014 Reported Amounts	Inventory-Defined Solubility Limit[a] (M)
Actinides					
^{225}Ac	1.25	2.16×10^{-8}	27.2 (3.60×10^{-4})	N/A	<< Solubility
^{227}Ac	25.9	3.60×10^{-4}			
^{229}Th	1.25	5.97×10^{-3}	46.3 (1.08×10^{3})	7.04 (1.35×10^{4})	>> Solubility
^{230}Th	2.66	0.127			
^{232}Th	0.119	1.08×10^{3}			
^{234}Th	42.3	1.84×10^{-6}			

Table 6. CRA-2019 WIPP Radionuclide Inventory Decay-Corrected to 2033 (Table CRA-2019 SOTERM -11).

Selected Radionuclides	Activity (Ci)	Amount (kg)	Element-Specific Inventory (all reported isotopes)	CRA-2014 Reported Amounts	Inventory-Defined Solubility Limit[a] (M)
^{233}U	1.27×10^{2}	13.1	663 (1.28×10^{5})	528 (2.26×10^{5})	>> Solubility
^{234}U	4.86×10^{2}	78.5			
^{235}U	6.41	2.91×10^{3}			
^{236}U	0.677	10.4			
^{238}U	42.3	1.25×10^{5}			
^{237}Np	34.4	48.5	469 (48.5)	23.2 (32.5)	8×10^{-6} M (≥ projected solubility)
^{239}Np	4.35×10^{2}	1.89×10^{-6}			
^{238}Pu	9.64×10^{5}	56.7	4.03×10^{6} (1.56×10^{4})	2.02×10^{6} (1.20×10^{4})	>> Solubility
^{239}Pu	8.74×10^{5}	1.41×10^{4}			
^{240}Pu	3.19×10^{5}	1.39×10^{3}			
^{241}Pu	1.87×10^{6}	18.7			
^{242}Pu	1.64×10^{2}	42.0			
^{244}Pu	3.40×10^{-2}	4.79			
^{241}Am	1.14×10^{6}	336	1.14×10^{6} (3.38×10^{2})	7.05×10^{5} (203)	5×10^{-5} M (≥ projected solubility)
^{243}Am	4.35×10^{2}	2.17			
^{244}Cm	3.94×10^{4}	0.486	3.99×10^{4} 2.13	9.97×10^{3} (0.122)	~ 3 x 10^{-8} M
^{246}Cm	5.10×10^{2}	1.64			
^{249}Cf	48.3	1.18×10^{-2}	48.3 (1.18×10^{-2})		
Fission Products[b]					
^{137}Cs	2.51×10^{5}	2.88	2.51×10^{5} (2.88)	2.35×10^{5} Ci 2.67 Kg	1×10^{-6} M
^{90}Sr	1.97×10^{5}	1.41	1.97×10^{5} (1.41)	2.09×10^{5} Ci 1.51 Kg	1×10^{-6} M

[a] Moles in the inventory divided by the minimum brine volume (17,400 m^3).

[b] Fission products are not TRU, but are considered in the PA to calculate overall release.

Table 7. Comparison of Inventory-limited Concentration and Projected Solubility for the Actinides (Table CRA-2019 SOTERM-24).

Actinide	Inventory at 2033 y (Kg)	Inventory-Defined Concentration (M)	[a]Calculated Mobile Concentration (M)	Ratio of Inventory to Calculated Concentration
Ac	3.6×10^{-4}	9.1×10^{-11}	5.12×10^{-7}	1.8×10^{-4}
Th	1.08×10^{-3}	2.7×10^{-4}	1.22×10^{-7}	2213
U	1.28×10^{5}	3.1×10^{-2}	1.0×10^{-3}	31
[b]Np	48.5	1.2×10^{-5}	1.32×10^{-6}	9.1
Pu	1.56×10^{4}	3.8×10^{-3}	5.12×10^{-7}	7422
[c]Am	338	8.1×10^{-5}	5.12×10^{-7}	158
Cm	2.13	5.0×10^{-7}	5.12×10^{-7}	1.02

[a]Calculated based on highest possible total mobile concentration (Domski 2019).
[b]Np increases in inventory and has a concentration ratio of 73.3 at 5000 y.
[c]Am is below inventory limit at 5000 y after emplacement.

5.2 Task 1: Experimental Plans/Approach to Challenge the An(III) WIPP Model

The An(III) oxidation state, which pertains to Pu(III) and Am/Cm(III), is the most important oxidation state from the perspective of potential release from the WIPP. In WIPP PA, plutonium and americium account for over 90% of the release throughout repository lifetime. An(III) oxidation state encompasses all the americium isotopes and 50% of the plutonium isotopes during the 10,000-y repository performance lifetime. It is important for this reason that the model for this oxidation be well supported scientifically. A review of this oxidation state in EPA response SOTERM-3 (Reed, 2021) established the following potential concerns in the current modeling approach:

a) There are new scientific data that update current scientific thinking regarding the key reactions and Log Ks used in the WIPP model. Consideration should be given to update the

currently accepted and internationally peer reviewed values recommended by the NEA-TDB (when available). This change would necessitate the recalculation of the associated Pitzer parameters.

b) The current WIPP approach and strategy for the $An(OH)_3$ solubility controlling phase continues to be an area of discussion within the WIPP project. The basis of the Giambalvo recommendation, which was to use a very low Log K of -27.5 for $Am(OH)_3$ (s), is no longer supported by the international community and seems to be inconsistent with most of the more recent literature data as well as the Nuclear Energy Agency (NEA) recommendations [it predicts a lower solubility than the currently accepted value for $Am(OH)_3$ (cr)]. Additionally, there are no recognized Pu(III) crystalline phases at pH> 6 although there are more recent data (Reed et al. 2012; Tasi et al. 2018) to support the persistence of this oxidation state under WIPP-relevant conditions. Given that the goal of the WIPP model is to realistically predict release under these expected conditions, it makes sense to strategically re-evaluate the use of the Log K values for the amorphous phases as this appears to be predominant in the simulated WIPP brine systems. Also, amorphous phases are generally observed in more broadly-based studies for Am/Nd (and the only phase that can be present for the more important plutonium system).

c) There are key questions about the formation constants for the complexation of An(III) with EDTA and citrate. In both cases, the Log Ks used for these organics appear to be underestimated by current modeling approaches and the data currently in the WIPP model. The data that support these values are somewhat unreliable, based on the original authors' opinions, and are not confirmed by the WIPP experimental results. For this reason, they should be re-evaluated experimentally as a function of ionic strength to determine the Log K and associated Pitzer interaction parameterizations.

d) It is unclear if the high pH speciation of the An(III) actinides is fully captured by the current WIPP model. Model fits of An(III) solubility under WIPP-relevant conditions (e.g., in WIPP simulated brines) should be assessed further experimentally, particularly with respect to 1) borate, and 2) EDTA/Citrate high-pH speciation effects.

The first and second items (a and b) are mainly modeling activities to evaluate the NEA-TDB data and the overall basis of the Pitzer parametrizations made by Giambalvo (2002a).

The third and fourth issues (c and d) just listed; however, require additional experiments. These form the basis of the research activities described in in Task 1.

The overall strategy is to complete and perform these model updates in the CRA-2024 timeframe. The benefit to the DOE-CBFO, when these data are combined with appropriate modeling activities, is that the following An(III) updates will be implemented:

a) High pH speciation will be assessed and speciation (solid and aqueous phase) appropriate to the expected WIPP environment, should brine inundation occur, will be confirmed.

b) Updated Log K and associated Pitzer interaction parameterizations will be established for the An(III)-citrate and An(III)-EDTA complexes.
c) The effects of borate on the speciation of An(III) will be incorporated into the model.

5.2.1 Subtask 1.1: Assessment of high pH speciation supporting the solubility of An(III) in WIPP brine

The first experimental question addressed is the high-pH speciation of An(III) in the presence of the EDTA and Citrate complexes. There are preliminary data (ACRSP unpublished) that suggest the 1:1 complex is stable up to pH ~ 10 for EDTA whereas the literature shows a potentially more complex speciation for the citrate complex (Reed 2021). These will be evaluated by monitoring the spectroscopy and solution concentration of the Am-EDTA or Citrate complex as a function of I (0.1 to 5 m) and up to a pH of 12. Changes in the speciation, if observed, will be evidenced by new band formation (further red-shifted) that change the overall spectra observed. If no change is observed, then this will confirm that the speciation is likely unchanged. This is a screening activity to assess the extent to which the 1:1 complex describes the high pH speciation of Am(III). If new speciation is observed, then the associated absorption spectroscopy will be assessed in a higher pH range for the two complexants. This will confirm/define the overall speciation approach used in Subtask 1.2.

The goal is to evaluate these effects to within a 10% change on the spectroscopically-determined speciation.

5.2.2 Subtask 1.2: Measurement of EDTA and Citrate An(III) formation constant as a function of Ionic Strength

An evaluation/confirmation of the effects of organics were performed to support the CRA-2009 as there were relatively few data for these key organic complexes. These results are shown in Figure 3 for GWB. In this evaluation, only citrate and EDTA had an effect on the apparent solubility of the $Nd(OH)_{3\,(am)}$ phase. In the case of ERDA-6 brine, there was a ~1:1 correlation between the concentration of EDTA and dissolved Nd. For GWB, the presence of magnesium reduced this to an ~ 1:2 ratio due to competition with the Mg^{2+} present. Neither of these effects are well predicted by the current WIPP model. For oxalate and acetate, there was no measurable enhancement of the Nd(III) solubility at WIPP-relevant concentrations although some oxalate precipitation effectively lowered the observed Nd concentration.

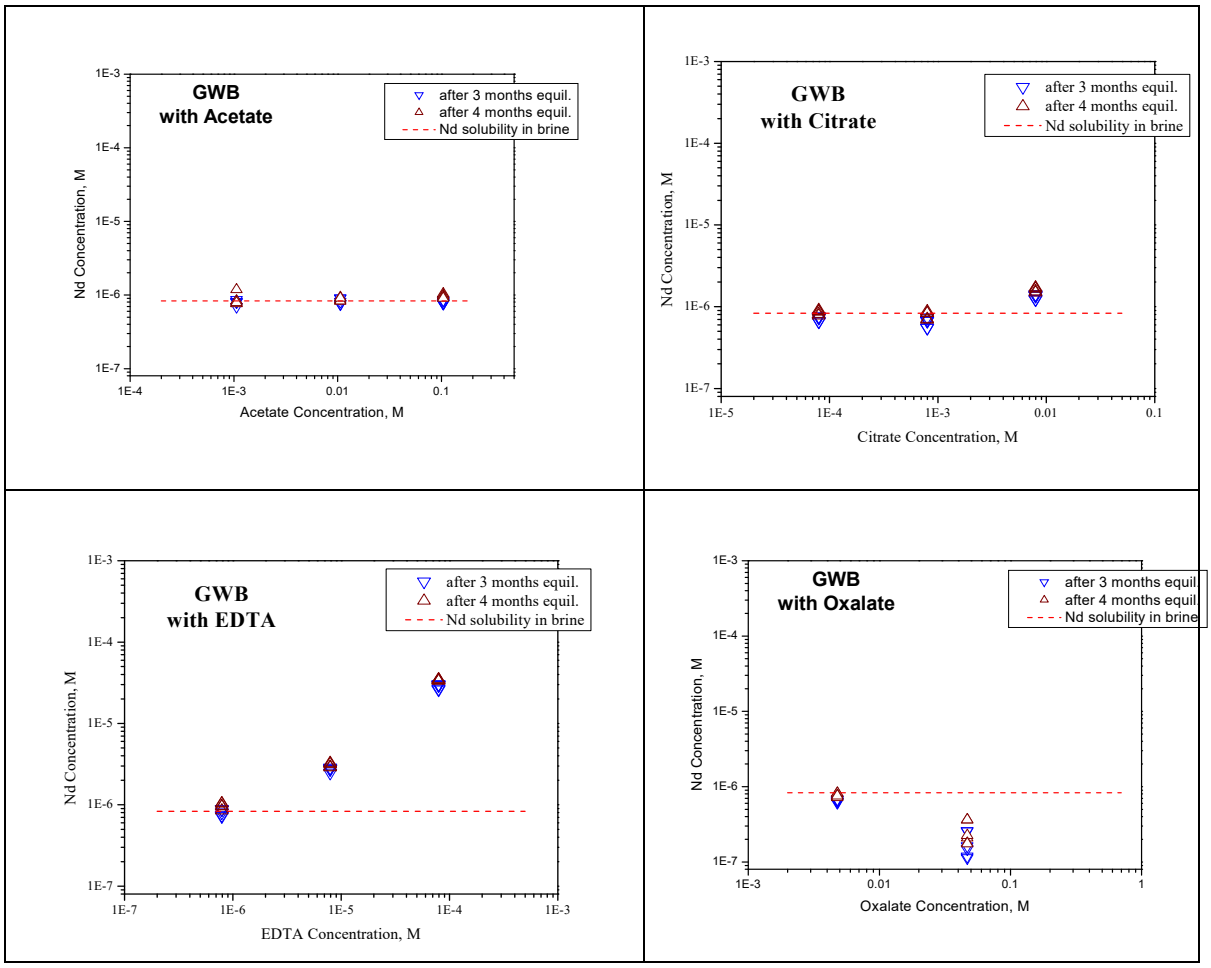


Figure 3. Effect of EDTA, Citrate, Oxalate and Acetate on the Solubility of Nd^{3+} in GWB Brine (Based on CRA-2014, Appendix SOTERM-21).

Americium [when compared to Pu(III) and Nd(III)] has a favorable spectroscopy for speciation studies meaning that complexation leads to new band formation that readily permits quantification. This is illustrated in Figure 4 for Am-EDTA. Complexation, in this system, leads to a ~ 4 nm red-shift and the measurement of this spectrum as a function of EDTA/Am ratio, pH and ionic strength will provide the needed data to determine the 1:1 Log K and the Pitzer parameters to model ionic strength effects. An analogous spectroscopy is expected for the Am-citrate complex. The test Matrices for EDTA and Citrate experiments are shown in Tables 8 and 9 respectively. The successful analysis of these data is expected to lead to a new QL1 determination of the Log K and associated Pitzer parameters for the EDTA and citrate complex.

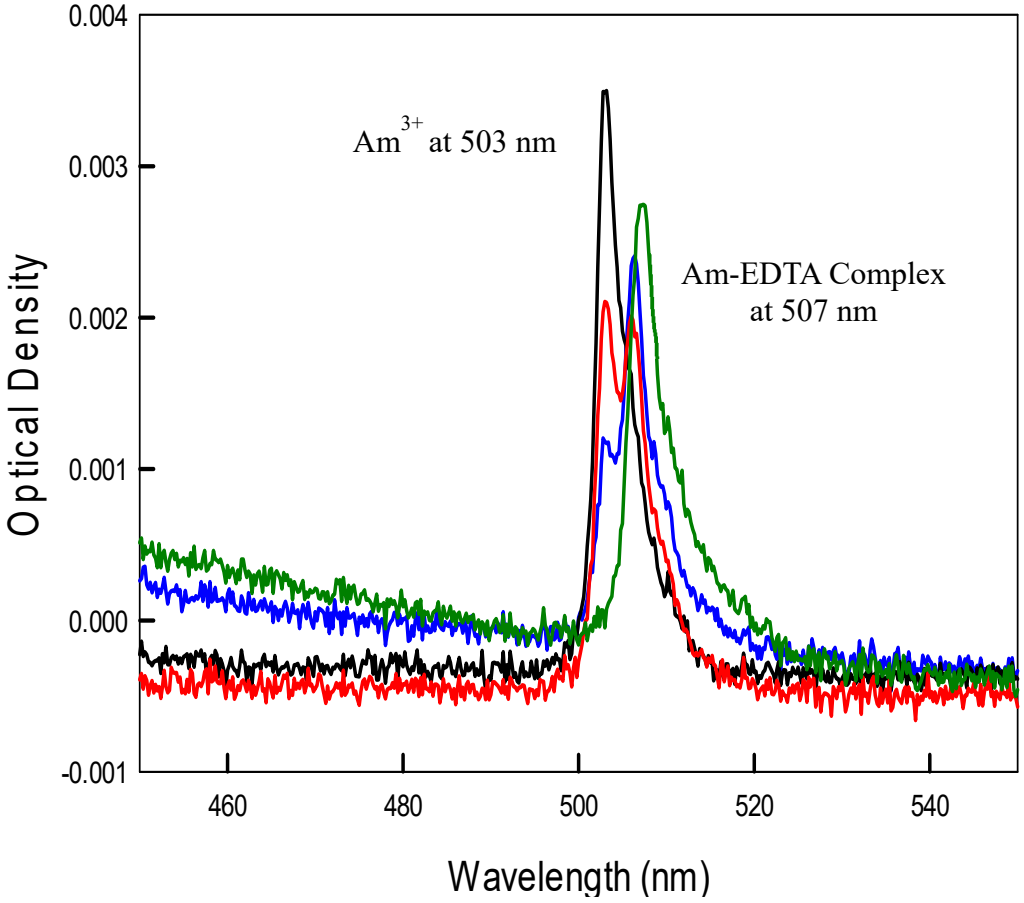


Figure 4. Effect of EDTA complexation on the absorption spectrum of Am^{3+}. Spectra were obtained at a fixed 0.1 mM EDTA as a function of pH (Black – aquo species; Red and Blue – pH ~ 1 and 3; Green – pH ~ 12).

Table 8. Experimental Matrix to Determine the Log K for the 1:1 Am-EDTA Complex (all at fixed temperature of 25 ± 0.2 ˚C).

Experiment Designation	Complexant	Ionic Strength [NaCl]	pH	L/M ratio	Comment
AmE-Low	EDTA	0.1 m	Variable 0.5 – 2.0	Variable 1-100	Evaluate L/M effect on speciation
AmE-High	EDTA	5.0 m	Variable 0.5 – 2.0	Variable 1-100	Evaluate L/M effect on speciation
AmE-I-01	EDTA	0.1	Variable 0.5 – 2.0	10*	Evaluate Log K at I = 0.1 m
AmE-I-05	EDTA	0.5	Variable 0.5 – 2.0	10*	Evaluate Log K at I = 0.5 m
AmE-I-1	EDTA	1.0	Variable 0.5 – 2.0	10*	Evaluate Log K at I = 1.0 m
AmE-I-2	EDTA	2.0	Variable 0.5 – 2.0	10*	Evaluate Log K at I = 2.0 m
AmE-I-3	EDTA	3.0	Variable 0.5 – 2.0	10*	Evaluate Log K at I = 3.0 m
AmE-I-4	EDTA	4.0	Variable 0.5 – 2.0	10*	Evaluate Log K at I = 4.0 m
AmE-I-5	EDTA	5.0	Variable 0.5 – 2.0	10*	Evaluate Log K at I = 5.0 m

*assumes 100% complexation (to be confirmed experimentally).

Table 9. Experimental Matrix to Determine the Log K for the 1:1 Am-Citrate Complex (all at fixed temperature of 25 ± 0.2 ˚C).

Experiment Designation	Complexant	Ionic Strength [NaCl]	pH	L/M ratio	Comment
AmC-Low	Citrate	0.1 m	Variable 0.5 – 2.0	Variable 1-100	Evaluate L/M effect on speciation
AmC-High	Citrate	5.0 m	Variable 0.5 – 2.0	Variable 1-100	Evaluate L/M effect on speciation
AmC-I-01	Citrate	0.1	Variable 0.5 – 2.0	10*	Evaluate Log K at I = 0.1 m
AmC-I-05	Citrate	0.5	Variable 0.5 – 2.0	10*	Evaluate Log K at I = 0.5 m
AmC-I-1	Citrate	1.0	Variable 0.5 – 2.0	10*	Evaluate Log K at I = 1.0 m
AmC-I-2	Citrate	2.0	Variable 0.5 – 2.0	10*	Evaluate Log K at I = 2.0 m
AmC-I-3	Citrate	3.0	Variable 0.5 – 2.0	10*	Evaluate Log K at I = 3.0 m
AmC-I-4	Citrate	4.0	Variable 0.5 – 2.0	10*	Evaluate Log K at I = 4.0 m
AmC-I-5	Citrate	5.0	Variable 0.5 – 2.0	10*	Evaluate Log K at I = 5.0 m

*assumes 100% complexation (to be confirmed experimentally).

5.2.3 Subtask 1.3: Effects of borate on An(III) solubility

The effect of borate on the apparent solubility of An(III) was already evaluated using Nd as an analog for Am(III) and Pu(III) (Borkowski et al. 2010a and 2010b). These data were obtained at a time when the borate chemistry was not as well understood and, in particular, the importance/role of the high concentration range of WIPP-relevant borate concentrations was not fully assessed experimentally. A re-assessment of these data is also needed for CRA-2024. Confirmatory studies in two areas may be needed: 1) Boron Nuclear Magnetic Resonance (NMR) at high borate concentration to confirm the speciation and 2) additional solubility data to

fully evaluate the borate effect (it is not likely that direct techniques can be used as the solubility in the presence of borate will likely be too low). The boron NMR will be performed at facilities located at LANL using samples prepared under the LANL-CO QA program. The solubility studies will be performed in ACRSP labs (Nd).

Boron NMR (if needed): These will confirm high borate concentration speciation.

[Borate] = 100 to 160 mM

pH: titration from pH < 4 to pH > 12

Additional solubility experiments (if needed): These will focus on the high end of the borate range found under WIPP-relevant conditions ([borate] > 100 mM):

Nd/Am(III) in the presence of variable borate concentrations under carbonate-free and anoxic conditions

Solids: $An(OH)_{3\ am}$

pH range: 7 – 12 (where borate effects predominate)

5.2.4 Subtask 1.4: Solubility of $An(OH)_{3\ am}$ and $An(OH)_{3\ cr}$ in the presence of Citrate and EDTA

Confirmatory solubility studies for both initially amorphous and crystalline phases of $An(OH)_3$ will be performed. These will be done in NaCl and simulated WIPP brine from an under-saturation approach. The goal of these studies is to support the directly determined formation constant measurement (Subtask 1.2 and, if needed 1.3) with measured solubilities to confirm the overall chemistry model and challenge the predictions of the Pitzer model for this system. The Test Matrix for these experiments is shown in Table 10. These experiments, due to curie (Ci) limitations at CEMRC, will most likely be performed at the University of Notre Dame (Professor Amy Hixon) directly assisted by ACRSP staff.

Table 10. Experimental Matrix to Challenge and Confirm An(III)* Solubility Model Predictions Using the EDTA and Citrate Results from Subtasks 1.1 and 1.2.

Experiment Designation	Solid Phase	Medium	[Complexant] in m	pC_{H+}	Comment
An-am-01-"pH"	$An(OH)_{3\ am}$	0.1 m NaCl	Inventory defined EDTA/ Citrate	7, 9, 11	Low I model challenge
An-am-5-"pH"	$An(OH)_{3\ am}$	5.0 m NaCl	Inventory defined EDTA/ Citrate	7, 9, 11	High I model challenge
An-cr-01-"pH"	$An(OH)_{3\ cr}$	0.1 m NaCl	Inventory defined EDTA/ Citrate	7, 9, 11	Low I model challenge
An-cr-5-"pH"	$An(OH)_{3\ cr}$	5.0 m NaCl	Inventory defined EDTA/ Citrate	7, 9, 11	High I model challenge
An-am-WIPP	$An(OH)_{3\ Am}$	pH-specific WIPP Brine	Inventory defined EDTA/ Citrate	7, 9, 11	High I model challenge

*An = Nd^{3+} and/or Am^{3+}

5.3 Task 2: Experimental Plans/Approach to Challenge the An(IV) WIPP Model

The An(IV) oxidation state WIPP solubility model currently uses Th(IV) as an analog for U(IV), Np(IV), and Pu(IV) speciation and solubility. This has been true since the time of the CCA and thorium is also widely used in this way for many of the high-level waste repository projects since it is redox invariant and only exists as Th(IV) in solution. Additionally, it has the key experimental advantage of being very low in activity meaning that it is easy to use in the lab.

There are, however, some significant limitations to using thorium as the An(IV) analog. Thorium chemistry is significantly different than U(IV), Np(IV) and Pu(IV) in that it has a much lower tendency to undergo hydrolysis which leads to an over-prediction of the solubility of the other actinides. Additionally, in the high ionic strength brine systems expected in the WIPP, the colloidal tendencies are also very different making it difficult to use as an analog for the An(IV) colloidal systems. Lastly, thorium has some analytical limitations. Because it is relatively low atomic number Z (compared to U, Np and Pu) it has a higher level of interferences in brine systems for ICP-MS analysis giving it a somewhat lower detection limit. Lastly, it does not have a favorable absorption spectroscopy meaning direct spectroscopic methods cannot be used for complex formation and speciation studies.

A review of the thorium database was performed as part of CRA-2019 as EPA response SOTERM-4 (Beam 2021). The key issues identified in this review were:

a) There appear to be many disconnects with the current scientific thinking regarding the key reactions and Log Ks used in the WIPP model. The WIPP should consider an update to the currently accepted and internationally peer-reviewed values recommended by the

NEA-TDB (when available). This change may necessitate the recalculation of the associated Pitzer parameters.

b) There are potentially some key limitations to the carbonate speciation in the WIPP model. Studies of Th(IV) in carbonate containing solutions identified five hydroxycarbonate complexes responsible for controlling the solubility of ThO_2(am) at high ionic strengths (Altmaier et al. 2004, Altmaier et al. 2006). Of these five complexes, only $Th(OH)_3(CO_3)^-$ is included in the WIPP An(IV) model. Reassessment of the solubility of ThO_2(am) as a function of carbonate concentration and pH will lead to a clearer understanding of the species that impact solubilization under WIPP conditions.

c) The WIPP model may not accurately define organic speciation. EDTA and citrate, two ligands expected to enhance the solubility of An(IV), have both been shown to form ternary species under high ionic strength and high pH conditions. $Th(OH)_2(EDTA)^{2-}$ and $Th(OH)_3(EDTA)^{3-}$ were both found to be important to describe the solubility of ThO_2(am) in the presence of EDTA (Xia et al. 2003). Four ternary citrate species were also found to be important to describe the behavior of ThO_2(am) in the presence of citrate (Felmy et al. 2006). Acetate and oxalate, while not expected to impact An(IV) solubility, have also been shown to form multi-ligand complexes with Th(IV) that are not represented in the WIPP An(IV) model.

d) The potential role of borate on An(IV) speciation is not addressed in the model. It is likely that borate is a non-factor since we would expect its chemistry to mirror carbonate and hydrolysis should predominate at the pH ~ 9 predicted for the WIPP. But the highly colloidal systems evaluated in past work has potentially masked the effects of borate. For this reason, there should be additional experimental confirmation that borate does not impact An(IV) speciation.

The first two issues just listed (a and b) are centered on carbonate speciation and hydrolysis speciation that will not be investigated experimentally in this Test Plan. This is mainly because sufficient literature data appears to exist for these two systems. There is, however, a need to confirm and/or re-assess the potential impacts of borate and organics (issues c and d) as these are not well addressed by the existing WIPP model.

The overall strategy is to evaluate the WIPP An(IV) model in two steps:

1) Assess and strengthen the WIPP thorium model. This will be done in a timeframe to support CRA-2024 with the goal of strengthening and more completely assessing the appropriateness of the current WIPP thorium model.

2) Evaluate the replacement of thorium as the analog for An(IV) with Np/U(IV). This will be done in the timeframe to support CRA-2029 with the goal of improving the overall accuracy and relevance of the An(IV) model to simulate Pu(IV) chemistry – which is the most important An(IV) actinide. The

experiments needed to do this shift will be developed at a later time using a TIP that provides the detailed plans for this key change.

The benefit to the DOE-CBFO in completing the research activities in Task 2 is that:

a) A stronger and more robust Th(IV) WIPP model will be available for implementation in CRA-2024.

b) A more accurate change from Th(IV) to Np/U(IV) as the analog for Pu(IV) will be available for CRA-2029.

5.3.1 Subtask 2.1: Assessment of the effects of organics on the WIPP Thorium An(IV) Model

Preliminary assessments of the effects of organics on thorium solubility were performed previously and concluded that there was little/no effect of organics (CRA-2014, Appendix SOTERM Section 3.8.2). These results, however, are no longer supported by recently obtained results (Yalcintas et al. 2019) that show a predominance of ternary species at high pH that appear to be a further hydrolysis of the 1:1 organic complex initially formed. The initial data obtained were masked by the colloidal speciation of thorium and were not done well enough (not enough equilibration time, and not from over-saturation).

In this subtask, the potential role of organics on An(IV) speciation will be evaluated from over and under saturation. The experimental matrix for these experiments is shown in Table 11.

Table 11. Experimental Matrix for the Thorium and Neptunium An(IV) Organic Screening Experiments.

Experiment	Organic Present	pC_{H+}	Brine System	Approach
Thorium Experiments				
Th-Control	None	7, 9, 11	pH specific simulated WIPP brines	Under-saturation
Th-ORG	EDTA, Citrate, Oxalate and Acetate	7, 9, 11	pH specific simulated WIPP brines	Under-saturation
Th-EDTA	EDTA	7, 9, 11	pH specific simulated WIPP brines	Over-saturation
Th-Citrate	Citrate	7, 9, 11	pH specific simulated WIPP brines	Over-saturation
Th-Oxalate	Oxalate	7, 9, 11	pH specific simulated WIPP brines	Over-saturation
Th-Acetate	Acetate	7, 9, 11	pH specific simulated WIPP brines	Over-saturation
Neptunium (IV) Experiments				
Np-Control	None	7, 9, 11	pH specific simulated WIPP brines	Under-saturation
Np-ORG	EDTA, Citrate, Oxalate and Acetate	7, 9, 11	pH specific simulated WIPP brines	Under-saturation
Np-EDTA	EDTA	7, 9, 11	pH specific simulated WIPP brines	Over-saturation
Np-Citrate	Citrate	7, 9, 11	pH specific simulated WIPP brines	Over-saturation
Np-Oxalate	Oxalate	7, 9, 11	pH specific simulated WIPP brines	Over-saturation
Np-Acetate	Acetate	7, 9, 11	pH specific simulated WIPP brines	Over-saturation

These will be done with thorium to directly support the current WIPP model, but also with Np(IV) using in-situ redox control methods to more accurately evaluate the likely effects on Pu(IV) chemistry.

5.3.2 Subtask 2.2: Assessment of the effects of borate on the solubility of An(IV)

In this subtask, it is expected to confirm that borate does not have a significant effect on the solubility of An(IV) actinides. This will be done using Th(IV) to obtain data that directly pertains to the current WIPP model but also with Np(IV) to more completely evaluate the potential effect that borate may have on the solubility of Pu(IV). The matrix for these experiments is given in Table 12. A precipitated hydrous amorphous phase will be used as the solubility-controlling solid phase.

Table 12. Experimental Matrix for the Thorium and Neptunium An(IV) Borate Screening Experiments.

Experiment	[Borate] in mM	pC_{H+}	Brine System	Approach
Thorium Experiments				
Th-B-C	0	9	pH specific simulated WIPP brines (modified)	Under-saturation
Th-B-25	25	9	pH specific simulated WIPP brines (modified)	Under-saturation
Th-B-50	50	9	pH specific simulated WIPP brines (modified)	Under-saturation
Th-B-100	100	9	pH specific simulated WIPP brines (modified)	Under-saturation
Th-B-WIPP	As-is Brine	9	pH specific simulated WIPP brines	Under-saturation
Neptunium (IV) Experiments				
Np-B-C	0	9	pH specific simulated WIPP brines (modified)	Under-saturation
Np-B-25	25	9	pH specific simulated WIPP brines (modified)	Under-saturation
Np-B-50	50	9	pH specific simulated WIPP brines (modified)	Under-saturation
Np-B-100	100	9	pH specific simulated WIPP brines (modified)	Under-saturation
Np-B-WIPP	As-is Brine	9	pH specific simulated WIPP brines	Under-saturation

5.3.3 Subtask 2.3 Use of Np(IV)/U(IV) as the basis of the WIPP An(IV) Model

Th(IV) has two major drawbacks when used as an analog of Pu(IV) behavior. The first of which is that Th(IV) is estimated to be ~ 100 times more soluble than Pu(IV). While this is

useful from a PA point of view, as releases are always over-predicted, it does not accurately represent Pu(IV) behavior. The second drawback is the high prevalence of metastable colloids that readily occurs in high ionic-strength Th(IV) systems (see discussion in CRA-2019, Appendix SOTERM, Section 5.4) that is not present in the other An(IV) species. These colloids are difficult to remove from solution and are metastable for several years, complicating the data analysis of all high ionic-strength An(IV) solubility studies.

U(IV) and Np(IV) have more similar behavior to Pu(IV) than Th(IV). This allows for them to be used to model Pu(IV) and achieve a more realistic depiction of the solubility and speciation of the Pu(IV) system. A detailed report outlining the use of U(IV) and Np(IV) as an analog for Pu(IV) was published in a WIPP-funded study by INE (Altmaier et al. 2017). Although some scoping experiments may be performed for CRA-2024, this subtask targets the CRA 2029 timeframe. In this context, a detailed TIP (according to ACP-IMP-007) will be written with the experimental details as this is a significant change/update to the WIPP actinide solubility model. The scope of the planned experiments will include:

a) The E_h range of U(IV) and Np(IV) systems under WIPP relevant conditions will be examined (presence of iron, tin, lead, and organics). This ties into current discussions about the Pu oxidation state distribution in the WIPP. If a defensible range of E_h values can be established, modeling will support an overall oxidation state distribution of the actinides of interest rather than the distributions currently chosen for PA applications.

b) U(IV) and Np(IV) experiments in simplified brine systems will be undertaken to determine formation constants and Pitzer parameters for systems relevant to WIPP conditions. These will eventually replace the less accurate Th(IV) model in WIPP PA.

5.4 Task 3: Experimental Plans/Approach to Challenge the An(V) WIPP Model

The WIPP An(V) solubility model is used to predict the solubility of Np(V) in the least reducing oxidation state distribution actinide set. Both americium and plutonium have An(V) species, but in both cases these are not predicted based on redox arguments. Because this model only supports Np(V), and Np has historically had a low projected inventory, it has been largely ignored since the CCA although the speciation model was updated in 2002 (Giambalvo 2002c). In CRA-2005, 2009 and 2014, the DOE argued that the potential contributions of Np (V) to release from WIPP could be excluded based on inventory arguments. As shown in Table 7, the current (CRA-2019) inventory of neptunium shows that there is now over nine times the predicted solubility of neptunium in the inventory. More importantly, this is the only TRU component that increases in the inventory with time as it is the main daughter product of Am-241 decay (alpha, n) so its relative importance increases throughout the 10,000-year performance period of the WIPP.

The $Np(V)O_2^+$ ion is the most stable ion in solution within the An(V) series. This valence stability of Np(V) in aqueous solution makes neptunium a useful representative element for studying the aqueous complex chemistry of all pentavalent actinides, but in the predicted WIPP scenario, as just discussed, it is only used to represent itself.

The currently predicted neptunium speciation is shown in Table 13. As indicated, this shows that acetate complexes (predominant), carbonate complexes and the aquo (uncomplexed) neptunyl species are the three most important species present. Although some solubility data exist (see reviews in CRA-2019 Appendix SOTERM, Section 5.6), these predictions have not been challenged experimentally under strictly WIPP relevant conditions. The overall strategy in this task is to experimentally challenge the model predictions using simulated WIPP brine and reassess the predicted model speciation to strengthen the overall WIPP An(V) model.

Table 13. Comparisons of Distributions of Dissolved Np(V) Species in the Minimum Volume of GWB and ERDA-6. Percentages of solubilities < 0.01 were not reported. The solubility-controlling solid was $KNpO_2CO_3$. (Domski and Sisk-Scott 2019).

Np(V) Species	GWB, minimum volume		ERDA-6, minimum volume	
	Concentration, M	% of Solubility	Concentration, M	% of Solubility
$NpO_2Ac(aq)$	2.35×10^{-07}	58.34	9.81×10^{-07}	81.50
NpO_2^+	7.05×10^{-08}	17.52	9.66×10^{-08}	8.02
$NpO_2CO_3^-$	6.48×10^{-08}	16.12	8.03×10^{-08}	6.67
NpO_2Ox^-	2.68×10^{-09}	6.66	3.36×10^{-08}	2.79
$NpO_2(OH)(aq)$	3.41×10^{-09}	0.85	$4.11\ E \times 10^{-09}$	0.34
NpO_2Cit^{2-}	1.40×10^{-09}	0.35	7.30×10^{-09}	0.61
$NpO_2(CO_3)_2^{3-}$	6.26×10^{-10}	0.16	8.51×10^{-10}	0.07
$NpO_2(OH)_2^-$	6.75×10^{-12}	-	7.89×10^{-12}	-
$NpO_2(CO_3)_3^{5-}$	3.61×10^{-12}	-	$7.54\ E \times 10^{-12}$	-
NpO_2EDTA^{3-}	8.04×10^{-15}	-	5.73×10^{-14}	-
NpO_2HEDTA^{2-}	2.70×10^{-17}	-	1.58×10^{-16}	-
$NpO_2H_2EDTA^-$	3.62×10^{-21}	-	2.18×10^{-21}	-
Total	4.02×10^{-07}	100	1.20×10^{-06}	100

A detailed literature review of the relevant organic, carbonate and hydrolysis data for the reactions in the WIPP model was recently completed (Aslani and Beam 2021). The key results of this review are:

a) Many of the Log Ks used in the WIPP model are also reviewed by the NEA and are in good agreement (within the uncertainty range) of the currently recommended values. The WIPP should consider strengthening the regulatory position of the WIPP by changing to the NEA-recommended values. This may require a re-estimation of the associated Pitzer interaction parameters.
b) More specifically for the organic complexants, the following were observed:
   - There is generally good agreement in the oxalate complexation values for NpO_2Ox^- with the NEA-TDB database except Patil (1978) and Maiwald (2020). For the complex of $NpO_2(Ox)_2^{3-}$ results coming from Patil (1978), the values are much higher than the NEA-TDB review.
   - For citrate complexation, there are only a few studies in the literature and the Pokrovsky's (1997) results are in a good agreement with the NEA-TDB.
   - The only data for EDTA complexation that can be compared with the NEA-TDB database is from Pokrovsky (1998). These results are in a good agreement with the NEA database.
   - In the NEA-TDB database, there are no selected data for acetate complexation. But the data in the literature are all in a good agreement.
c) There is no confirmation of the Pitzer parameters and many are estimated by analogy. This appears to an area where the current WIPP model could be improved. Newer literature should be evaluated in this context.
d) The WIPP model does not include ternary calcium species although these exist in the ThermoChimie and THEREDA data bases. The relevance of these calcium ternary species should be evaluated for the WIPP.
e) There are no borate reactions in the WIPP model although borate has been shown to complex Np(V) (Hinz et al. 2020; ACRSP unpublished data).
f) Spectroscopy appears to be a good experimental approach for the measurement of organic complexation of neptunium and was used in many of the organic complexation studies found.
g) There are no confirmatory studies in WIPP-relevant brine systems for the predicted speciation. This confirmation alone will greatly strengthen and improve confidence in the WIPP model and will help assess the relative importance of the organic speciation in defining the predicted solubility.

Observations a, b and c are outside the scope of this Test Plan. Observations d, e, f and g are addressed in the experiments proposed herein and specifically emphasize the organic complexation of neptunium (V). Three subtasks are identified:

Subtask 3.1: Screening experiments with organic complexants will be performed to confirm model predictions. This will be done with all organics together to establish the overall impact of the WIPP-relevant concentrations on the solubility. Additionally, each organic chelating agent will be investigated to establish their contribution to solubility and see if this is captured by current modeling correctly (all somewhat qualitatively). All of this will be done using pH-specific brines (procedure ACP-EXP-001) concurrently.

Subtask 3.2: Screening experiments to evaluate the relative impacts on neptunium solubility of carbonate and borate will be performed. These will be done in simplified brines with and without variable borate and carbonate concentrations.

Subtask 3.3: Experiments as a function of pH in pH-specific brines under fully WIPP-relevant conditions will be performed to establish the solubility controlling phase. This will be done from under-saturation with the predicted range of solids in the WIPP.

5.4.1. Subtask 3.1: Apparent Solubility of Np(V) under WIPP-relevant Conditions

A series of experiments that confirm/challenge the current model predictions for the apparent solubility of Np(V) in WIPP relevant brines will be performed. These will put in place needed baseline data for the An(V) oxidation state. All will be performed in simulated WIPP brine (see procedure ACP-EXP-001) for a period of up to six months using prior-established procedures (See Test Plans LCO-ACP-02, LCO-ACP-03, and LCO-ACP-07).

The test matrix for these experiments is shown in Table 14. Apparent solubilities will be measured in the absence/presence of carbonate, borate, and organics as a function of pH in pH-specific brines. Concentration measurement that support this subtask will be done to within ± 20% and all solubility data are “order of magnitude”.

5.4.2 Subtask 3.2: Screening Experiments with Organic Complexants to Confirm Model Predictions

The complexation of Np(V) with organics has been investigated in relatively few studies (Aslani and Beam 2021). The most important organic complexants for the WIPP are EDTA, citrate, oxalate and acetate. The predominant speciation of the An(V) in WIPP is based on current modeling assumptions, acetate complex followed by the aquo species, the carbonato complex and organic complexes. EDTA and citrate, in contrast to the other actinide complexes, are minor contributors to the source term speciation based on the current WIPP model (see Table 13).

Table 14. Matrix for WIPP-relevant Apparent Solubility of Np(V).					
Experiment Designation	**Solid Phase**	**Medium**	**Complexant**	**pC_{H+}**	**Comment**
Np5-Brine	Amorphous*	WIPP pH-specific brine	None	7, 9, 11	Carbonate and organic - free control
Np5-Organic	Amorphous*	WIPP pH-specific brine	Inventory-defined organics	7, 9, 11	Organic Effects Challenge
Np5-Carbonate	Amorphous*	WIPP pH-specific brine	1, 5 and 10 mM carbonate	7, 9, 11	Carbonate Effects Challenge
Np5-All	Amorphous*	WIPP pH-specific brine	WIPP-relevant organics and carbonate	7, 9, 11	Full Repository Conditions Challenge
*Amorphous phase of Np(V) precipitated in GWB brine					

In this subtask, the contributions of each organic under WIPP-relevant conditions will be evaluated. These will be done in a simplified 5 m NaCl brine to focus the contributions of the organic complexation with a confirmatory study in a WIPP relevant brine that accounts for brine component effects on the availability of the organics for complexation of Np(V) (i.e. account for competition for the organics). The matrix for these experiments is given in Table 15.

All experiments will be conducted in room temperature i.e., 22 ± 3°C. A simulated brine (pC_{H+} = 9 WIPP brine) and 5 m sodium chloride will be prepared according to existing procedures. The aqueous phase analysis of neptunium will be performed by ICP-MS. Ion chromatography will be used to measure organic concentrations and UV-Vis-NIR spectroscopy will be used to establish the aqueous speciation. All experiments will be performed in glove boxes to control the atmosphere although fume hoods designated for radioactive work will be used to prepare the initial stock solutions used. After steady-state is achieved, the organics (EDTA, oxalate, acetate, and citrate) will be added at the maximum 1X concentrations predicted for the WIPP. These will be added together individually to fully evaluate the contribution of each.

Table 15. Np(V) Organic Screening Studies on WIPP-relevant Solubility Effects.				
Experiment Designation	**Organic Complexant**	**Medium**	**pC_{H+}**	**Comment**
Np5-Control	None	5 m NaCl	7, 9, 11	NaCl (5m) control
Np5-Ac-N	Acetate	5 m NaCl	7, 9, 11	NaCl (5m) Effects
Np5-Ac-W	Acetate	pC_{H+} = 9 Brine	9	WIPP brine Effects
Np5-Ox-N	Oxalate	5 m NaCl	7, 9, 11	NaCl (5m) Effects
Np5-Ox-W	Oxalate	pC_{H+} = 9 Brine	9	WIPP brine Effects
Np5-Cit-N	Citrate	5 m NaCl	7, 9, 11	NaCl (5m) Effects
Np5-Cit-W	Citrate	pC_{H+} = 9 Brine	9	WIPP brine Effects
Np5-E-N	EDTA	5 m NaCl	7, 9, 11	NaCl (5m) Effects
Np5-E-W	EDTA	pC_{H+} = 9 Brine	9	WIPP brine Effects
Np5-ORG-N	All	5 m NaCl	7, 9, 11	NaCl (5m) Effects
Np5-ORG-W	All	pC_{H+} = 9 Brine	9	WIPP brine Effects

5.4.3. Subtask 3.3: Relative impacts of carbonate and borate

Neptunium complexation by carbonate has been investigated by others, and a number of solid phases have been proposed for solubility control (Aslani and Beam 2021). The effects of borate on Np(V) speciation were also observed in preliminary experiments performed (ACRSP unpublished experiments). The key research questions are if these complexants, under the predicted WIPP conditions, can predominate over the organic speciation addressed in Subtask 3.2. In this subtask, the goal is to determine the overall effects of borate and carbonate on the apparent solubility of Np(V), and establish the relative effects of this speciation on the overall brine systems expected. The matrix for these experiments is shown in Table 16.

For the anoxic, reducing, and mildly basic brine systems expected in the WIPP, the most important inorganic complexants are expected to be carbonate/bicarbonate and hydroxide. The major elements in the Salado and Castile brines are sodium [Na^+], calcium [Ca^{2+}], magnesium [Mg^{2+}], potassium [K^+], chloride [Cl^-], carbonate [CO_3^{2-}], hydrogen sulfide [HS^-], and borate [$B(OH)_3$] (brackets indicate basis species used for thermodynamic modeling). Borate concentration is much higher than the carbonate in WIPP brine so may mask the effects of carbonate.

Table 16. Np(V) Borate and Carbonate Studies on WIPP-relevant Solubility Effects.				
Experiment Designation	**Complexant**	**Medium**	**pC_{H+}**	**Comment**
Control				
Np5-C	No borate or Carbonate	5 m NaCl	7, 9, 11	Control
Borate Effects				
Np5-B-10	10 mM borate	5 m NaCl	7, 9, 11	Borate effects
Np5-B-50	50 mM borate	5 m NaCl	7, 9, 11	Borate effects
Np5-B-100	100 mM borate	5 m NaCl	7, 9, 11	Borate effects
Np5-B-WIPP	As-is in Brine	pC_{H+} Specific Brine	7, 9, 11	WIPP-relevant effects
Carbonate Effects				
Np5-C-1	1 mM carbonate	5 m NaCl	7, 9, 11	Carbonate effects
Np5-C-5	5 mM carbonate	5 m NaCl	7, 9, 11	Carbonate effects
Np5-C-10	10 mM carbonate	5 m NaCl	7, 9, 11	Carbonate effects
Np5-C-100	100 mM carbonate	5 m NaCl	7, 9, 11	Carbonate effects
Np5-C-WIPP	1 mM	pC_{H+} specific Brine	7, 9, 11	WIPP-relevant effects

All experiments will be conducted at room temperature i.e., 22 ± 3°C. Simulated brines and one simplified brine (sodium chloride) will be prepared according to existing procedures. The aqueous phase analysis of neptunium will be performed by ICP-MS, IC, and UV-Vis-NIR spectroscopy. The experiments will be performed in glove boxes designated for radioactive work. All will be done from an under-saturated approach using an Np WIPP brine-precipitated amorphous solid phase.

5.4.4 Subtask 3.4 – Np(V) Solubility Controlling Phase

There are a number of carbonate phases that are included in the WIPP model. Currently, the predicted solubility controlling phase is the potassium neptunyl carbonate solid phase ($KNpO_2CO_3$). But the model includes other phases as well. In this subtask, the solids in the WIPP model will be prepared and equilibrated in simulated WIPP brine to evaluate their long-term stability, and solubility. The experimental matrix for these experiments is given in Table 17. All of these will be performed in simulated WIPP brine, in a controlled temperature anoxic glovebox, using an under-saturation approach.

Table 17: Np(V) Solid Phase Stability Evaluation			
Experiment Designation	**Solid Phase**	**Medium**	**pH**
Np5-K	$KNpO_2(CO_3)$	pC_{H+} Specific Brine	9
Np5-K3	$K_3NpO_2(CO_3)_2$	pC_{H+} Specific Brine	9
Np5-Na	$NaNpO_2(CO_3)\cdot 3.5\ H_2O$	pC_{H+} Specific Brine	9
Np5-Na3	$Na_3NpO_2(CO_3)_2$	pC_{H+} Specific Brine	9
Np5-OH	$NpO_2(OH)$ (am, fresh)	pC_{H+} Specific Brine	9

5.5 Task 4: Experimental Plans/Approach to Challenge the An(VI) WIPP Model

The WIPP does not currently have an An(VI) solubility model. This model would pertain to uranium since Pu(VI) and Np(VI) are not expected under WIPP-relevant conditions. In the absence of a model, per agreement with the EPA, the concentration of uranium was set to be equal to a conservatively high 1 mM within the actinide source term model in 2005 (U.S. EPA 2005). This concentration replaced the 8.7×10^{-6} M (see Table 1) that was used in the CCA. The specific issue raised by the EPA was the lack of uranium carbonate data and their speculation that very high concentrations of uranium, due to carbonate complexation, were possible under WIPP-relevant conditions.

The assumed 1 mM solubility is the basis of the calculated colloidal contributions from uranium (VI) that is used to generate the An(VI) contribution to the mobile actinide source term used in the current PA approach. For this reason, uranium is the only oxidation state that shows up significantly in the Culebra as potentially transportable.

There are already some WIPP-relevant uranium solubility data. The brine-specific solubility of uranium was first determined at Argonne National Laboratory (Hobart and Moore 1996) which was part of the model-challenge research performed as part of the ASTP program and was the basis of the recommended values in the CCA. Since the CCA, the apparent solubility in GWB and ERDA-6 WIPP brines was measured in the presence and absence of carbonate (Los Alamos Test Plan LCO-ACP-02; Lucchini et al. 2010). These data are shown in Figure 5 and along with the pre-CCA data, show that the carbonate levels expected in the WIPP will not lead to the kinds of effects hypothesized by the EPA (by almost a factor of 100 to 1000). More importantly, for this Test Plan, an An(VI) Pitzer model that accounts for carbonate was added to the THEREDA database and the predicted effects of carbonate are confirmed to be much lower than speculated in the 2005 DOE-EPA agreement. The calculated total uranium concentration at $pC_{H+} \sim 9$ was 3.5×10^{-8} M (performed using the GWB code) and shows the predominant speciation under these conditions to be the hydroxide complexes. This calculation,

importantly, does not account for borate and organic complexation effects (since these are not in the THEREDA model) and were not considered in the 2005 EPA discussion about carbonate.

The imposed 1 mM solubility requirement by the EPA in 2005 is a good example of the model distortion that can occur when there is a lack of sufficient data. But, as just pointed out, this is no longer true and, in fact, a model does now exist that can explicitly address carbonate speciation in high ionic strength brines. The recommended path forward for the development of an An(VI) (uranium) model is the following:

1) Use the developed hydrolysis/carbonate Pitzer model (THEREDA) as the starting point for the WIPP model. That this model exists means that adequate supporting data and studies, developed outside the WIPP project, exist and sufficiently support a defensible hydrolysis/carbonate uranium model.
2) Address the missing gaps specific to the WIPP repository case in the THEREDA model experimentally. Specifically, there are two key interactions that are important in WIPP that are missing in the current THEREDA implementation:
    a. Borate effects are not considered. LANL has already shown that borate can impact uranium (VI) solubility. This was confirmed spectroscopically in some preliminary Pu(VI) studies where two borate complexes were observed. The extent that this occurs needs to be evaluated under the expected WIPP conditions.
    b. Organic interactions were not considered as these data are absent. There are WIPP data (Reed et al. 1997), but also an expectation from the literature that organic complexation will enhance uranium (VI) solubility. The extent that this occurs needs to be evaluated under the currently expected WIPP conditions.
3) To complete a WIPP An(VI) uranium model, the proper dependencies for borate and organic complexation will need to be added to the THEREDA An(VI) model. This is a more extensive activity that will require a detailed study.

The first action identified above would be a modeling activity and is outside the scope of this Test Plan. The second and third activity are the needed experiments to develop a WIPP specific An(VI) model and are briefly described in this Test Plan in the following two subtasks:

Subtask 4.1: Effects of borate and organics on the solubility of U(VI) for the expected conditions in the WIPP

Subtask 4.2: Thermodynamic data and model for the effects of borate and organic complexants on uranium (VI)

For CRA-2024, the goal is to complete subtask 4.1 as a screening activity. This will provide baseline solubility concentrations that account for the most important interactions expected under the predicted WIPP conditions. Subtask 4.2 is deferred to CRA 2029 and is conditional on DOE concurrence to complete the task of developing a WIPP An(VI) model.

The completion of this task directly benefits the DOE by generating the data needed for a strong and defensible argument to lower the "conservatively high" estimate of the concentration of uranium. This could replace the currently imposed 1 mM concentration used in PA and will be documented in the parameter recommendation report that supports CRA-2024.

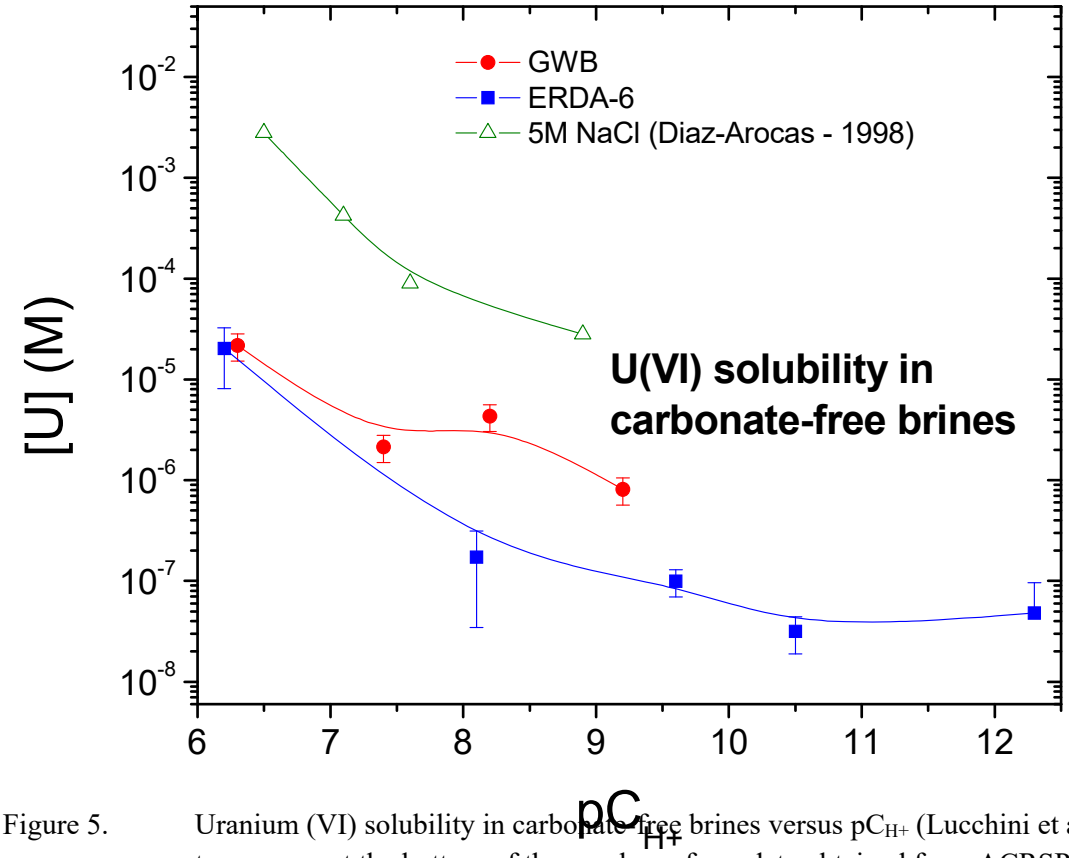


Figure 5. Uranium (VI) solubility in carbonate-free brines versus pC_{H+} (Lucchini et al. 2010). The two curves at the bottom of the graph are from data obtained from ACRSP solubility experiments in GWB (curve in the middle of the graph) and in ERDA-6 (curve at the bottom of the graph) using the over-saturation approach and the under-saturation approach. The top curve is based on the Diaz-Arocas' data in 5 M NaCl.

5.5.1 Subtask 4.1: Effects of borate and organics on the solubility of U(VI) for the expected conditions in the WIPP

The goal of this subtask is to perform screening experiments that account for the contributions of organics and borate to the observed WIPP-relevant uranium concentrations. This will evaluate the validity of the current 1 mM concentration assumption with a full consideration of the key factors that define the predicted concentration of uranium in the WIPP. The experimental matrix for these experiments is given in Table 18. These experiments will be

performed from an under-saturation approach using precipitated amorphous U(VI) hydroxide phases to define solubility.

Table 18. U(VI) Borate and Organic Screening Studies to Establish WIPP-relevant Solubility Effects.

Experiment Designation	Complexant	Medium	pC_{H+}	Comment
Borate Effects				
U6-B-0	0 mM borate	pC_{H+} Specific Brine*	9	Control
U6-B-10	10 mM borate	pC_{H+} Specific Brine*	9	Borate effects
U6-B-50	50 mM borate	pC_{H+} Specific Brine*	9	Borate effects
U6-B-100	100 mM borate	pC_{H+} Specific Brine*	9	Borate effects
U6-B-WIPP	Brine	pC_{H+} Specific Brine	9	WIPP-relevance
Organic Effects				
U6-ORG-C	No Organics	pC_{H+} specific Brine	9	Control
U6-ORG-AC	Acetate**	pC_{H+} specific Brine	9	Organic effects
U6-ORG-OX	Oxalate**	pC_{H+} specific Brine	9	Organic effects
U6-ORG-CIT	Citrate**	pC_{H+} specific Brine	9	Organic effects
U6-ORG-EDTA	EDTA**	pC_{H+} specific Brine	9	Organic effects
U6-ORG-WIPP	All Organics**	pC_{H+} specific Brine	9	WIPP-relevance

*pH-specific brine at pC_{H+} = 9 w/o borate
**at the predicted maximum 1 X concentration in CRA-2019

5.5.2 Subtask 4.2: Thermodynamic data and model for the effects of borate and organic complexants on uranium (VI)

The goal of this subtask is to obtain data to fully develop a thermodynamic model for borate and organic effects on U(VI) speciation and solubility. This is not planned for CRA-2024 and will be developed using a TIP if a decision is made to go forward with this activity.

6.0 Record Requirements

6.1 Record Generation and Maintenance

The following QA records are generated as a result of implementing this Test Plan. The records will be prepared and submitted to the LANL-CO Record Center in accordance with LANL-CO Quality Procedure LCO-QP17-1, Record Management.

Table 19. List of records generated.

Record	Originator	Record Submitter
Entries into task-specific scientific notebooks	Originator	ACRSP project leader or designate
Reports, publications, summaries of the data	Originator	ACRSP project leader or designate
Data Packages	Originator	ACRSP project leader or designate
Task Implementation Plans (Generated at the request of the Team Leader)	Originator	ACRSP project leader or designate

All documents generated by this Test Plan will be converted to lifetime records that will be retained for the lifetime of the project.

7.0 Attachments and Appendices

Not applicable as there are no attachments and appendices to this Test Plan.

8.0 Training and Qualifications

LANL-CO project participants will perform the work proposed in this Test Plan at the CEMRC facility and will be trained according to the training requirements established in LCO-QP-2-3. Read and sign training on this Test Plan will be documented according to LCO-QP2-3.