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Sandia National Laboratories
Waste Isolation Pilot Plant

Test Plan TP 20-01

Solubility and Complexation of Lead in Non-Sulfidic Brines of WIPP-Relevance

Task 4.4.2.2.1

Revision 0

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TABLE OF CONTENTS

ABBREVIATIONS, ACRONYMS AND INITIALISMS 4
1 REVISION HISTORY 5
2 PURPOSE AND SCOPE 5
3 EXPERIMENTAL PROCESS DESCRIPTION 7
3.1 Task List 8
3.1.1 Task 1: Synthesize and Characterize Solid Starting Materials 8
3.1.2 Task 2: Long-term Solubility Experiments 9
3.1.3 Task 3: Scoping Experiments 12
3.2 Overall Strategy and Process 14
3.3 Sample Control 16
3.4 Data Quality Control 16
3.4.1 Measuring and Test Equipment (M&TE) 16
3.4.2 Data Acquisition System 16
3.5 Data Identification and Use 17
3.6 Equipment and Techniques 17
3.6.1 Weighing Equipment 17
3.6.2 Liquid Measuring Equipment 18
3.6.3 Temperature Control Equipment 18
3.6.4 Other Analytical Equipment & Techniques 18
3.7 Records 18
3.7.1 Required QA Records 19
3.7.2 Miscellaneous Non-QA Records 19
4 TRAINING 19
5 HEALTH AND SAFETY 19
6 PERMITTING/LICENSING 20
7 REFERENCES 20

ABBREVIATIONS, ACRONYMS AND INITIALISMS

10X	10 times
ACS	American Chemical Society
AP	Analysis Plan
AR	Analysis Report
ASAP	Accelerated Surface Area and Porosimetry
ASTM	American Society for Testing and Materials
BET	Brunauer-Emmett-Teller
CPG	Carlsbad Programs Group
CRA	Compliance Recertification Application
DAS	Data Acquisition System
DI	Deionized
DOE	Department of Energy
DRC	Document Review Comment
DSC	Differential Scanning Calorimetry
EDS	Energy Dispersion Spectrometer
EDTA	Ethylenediaminetetraacetic acid
ERDA-6	Energy Research and Development Administration well 6 (Synthetic Castile Formation brine)
ES&H	Environmental Safety and Health
g	Gram
GWB	Generic Weep Brine (Synthetic Salado Formation brine)
IC	Ion Chromatography
ICP-AES	Inductively Coupled Plasma Atomic Emission Spectrometer
ICP-MS	Inductively Coupled Plasma Mass Spectrometer
kg	Kilogram
M&TE	Measuring and Test Equipment
m	molality, or mol/kg
mL	Milliliter
mol/L	mol per liter of solution
MOW	Member of Workforce
NIST	National Institute of Standards and Technology

NP	Nuclear Waste Management Procedure
PA	Performance Assessment
PAIR	Performance Assessment Inventory Report
PIP	Pitzer Interaction Parameter
ppm	parts per million
QA	Quality Assurance
RH	Remote Handled
s	solid phase
SEM	Scanning Electron Microscope
SNL	Sandia National Laboratories
SOP	Standard Operating Procedure
SP	Specific Procedure
TGA	Thermal Gravimetric Analysis
TP	Test Plan
µm	Micrometer
UV-Vis	Ultraviolet-Visible Spectrophotometer
WIPP	Waste Isolation Pilot Plant
XRD	X-Ray Diffractometer

1 REVISION HISTORY

This is the original version of this test plan. Revisions to this test plan will be prepared in accordance with the appropriate SNL WIPP Nuclear Waste Management Procedures (NPs).

For all procedures listed in this document, the most current revision of the document will be used for data collection.

2 PURPOSE AND SCOPE

WIPP performance assessment (PA) uses the actinide baseline solubilities calculated using the Pitzer activity-coefficient model for the various aqueous species of the WIPP relevant brines. The purpose of this test plan (TP) is to determine solution chemistry parameters for the solubility and complexation of lead in the WIPP relevant brines in non-sulfide systems. A previous TP 08-02 was initiated in 2008 for this purpose (Ismail et al., 2008), however, upon conducting final solid characterization of the experiments, lead solids were found to be different from the lead solid used to initiate those experiments. Lead solids, such as abellaite ($NaPb_2(CO_3)_2(OH)$), blixite ($Pb_8O_5(OH)_2Cl_4$), and laurionite ($PbCl(OH)$) were unexpectedly identified and documented (Kirkes et al., 2019) as “unexpected” because they were not in the thermodynamic database used to perform modeling. The observation of the “unexpected” lead solids indicates that we need to

determine the solubility of the solids to improve our model prediction capability by performing analytical and sequential experiments for the solids, as well as by referring to the literature information. The solubility and solid analysis from these new experiments in this test plan will be used to update the thermodynamic database to include the missing solids and associated information.

Upon collection of data from this TP, previous solubility data obtained under TP 08-02 will be compared with the data collected under this TP. For this purpose, a new Analysis Plan (AP) will be developed and an Analysis Report (AR) will be produced.

The decision to utilize lead shielding for Remote Handled (RH) waste containers sent to WIPP increases the lead inventory in the repository significantly. As of the cut-off date for the Performance Assessment Inventory Report 2012 (PAIR-2012), total projected lead in the waste packaging was 8.28×10^3 kg (Van Soest, 2012). After this cut-off date, 9 shielded containers were emplaced in the WIPP and additional shielded containers are expected to be emplaced before WIPP closure. This has led to an increase in lead volumes projected in the 2018 WIPP inventory report, with an estimate of 1.38×10^7 kg (Van Soest, 2018). Because of the increase in the WIPP lead inventory the total dissolved lead concentration of lead could affect repository performance. Therefore, the importance of determining accurate Pitzer interaction parameters (PIPs) and solubility constants for lead phases and species in WIPP relevant brines is a crucial aspect. The current database for the Pitzer thermodynamic model needs incorporation of those lead species in order to help reduce the uncertainty embedded in the actinide baseline solubility. To determine PIPs, simple and representative systems should be started by considering WIPP relevant brine conditions. Relevant lead solids are selected for combination with simple brine systems for long term solubility studies.

The purpose of the experimental work described in tasks 1 and 2 are to synthesize or purchase lead solids and then measure the solubilities of the lead solids in WIPP relevant brines. Experiments will be conducted under controlled environmental conditions (in a glove box). These solubilities, along with previously collected data will be used to determine the reaction constants and PIPs that will be incorporated into the WIPP thermodynamic database under a new AP. The experimental methodology will be used to measure the concentrations of components as functions of ionic strength of the solution and aging time. Brine solutions (such as magnesium chloride, sodium chloride, and mixtures of both) will be prepared and then lead solids to be studied will be introduced into the prepared brine solutions. Ionic strength, brine concentrations, pH and other parameters may be varied in order to investigate solubilities to develop new or verify the existing WIPP aqueous thermodynamic model for lead. The time-dependent measurements would ensure that system equilibria have been attained. Characterization of the solubility-limiting solids will be conducted and monitored for changes concurrently with the solution chemistry study as a function of time. In previous work, solid characterization was typically conducted at initiation and termination of the experiments, while in this study, solid characterization will be conducted simultaneously with each solution collection. Section 3.1.2 (task 2) discusses the set-ups of the long-term solubility experiments.

Task 3 will focus on the solubility of $PbCl_2$ in brines made of HCl, NaOH, NaCl, and $MgCl_2$. The complexation of lead with EDTA will also be investigated in task 3 to develop an aqueous thermodynamic database of lead under the Pitzer activity-coefficient model.

A better understanding of $PbCl_2$ solubility would enable us to elucidate the complexation of lead with other ligands such as, EDTA. Pb^{2+} may form species with organics (such as EDTA). Complexation of lead with EDTA could result in a possible reduction of actinide solubility in WIPP (U.S. DOE, 2019). Thus, the refined $PbCl_2$ solubility will contribute to the calculation of actinide baseline solubility in WIPP PA. The solubilities of $PbCl_2$ at different pH and the total chloride concentration up to 6.5 mol/L were measured previously by Noyes (1892), Armstrong and Eyre (1913), Herz et al. (1923), Kendall and Sloan (1925), Deacon (1927), Lewin et al. (1953), Tan et al. (1987), Holdich and Lawson (1987), Mgaidi et al. (1991), and Hagemann (1999). However, those experimental data show a noticeable data scatter among different measurements. von Ende (1901) measured the solubility of $PbCl_2$ in a chloride matrix up to 12 mol/L and they have a larger scatter, as the chloride concentration approach to high chloride concentration range. Moreover, there is a debate on which lead solid phases forms at higher chloride concentrations (Kendall and Sloan, 1925; Mgaidi et al., 1991). To cover WIPP relevant conditions, the solubility of $PbCl_2$ in chloride concentrations (up to the solubility limit of the selected background salts) will be measured in the brines containing NaCl and $MgCl_2$.

The results collected from this test plan will enable us to better understand the previous experimental data and will help determine the formation conditions of lead solids in WIPP relevant brines.

To gain a better modeling of the chemistry of the brines resulting in the lead solid transformation, the PIPs and the thermodynamic model need to be refined and extended so that the current thermodynamic database can be applied to represent both liquid chemistry and formation and/or transformation of relevant solids. Previous studies (Mgaidi et al., 1991; Felmy et al., 2000; Powell et al., 2009; Christov, 2009; and May and Rowland, 2017) have showed the modeling of the solubility of lead systems at various brine conditions. However, these modeling did not obtain a good representation of lead solids at high concentration of chloride. The complexation of aqueous species and solubility of lead solids, including solid identification will be determined in this TP. Results containing lead in aqueous form from the literature (Noyes, 1892; Armstrong and Eyre, 1913; Herz et al., 1923; Kendall and Sloan, 1925; Deacon, 1927; Lewin et al., 1953; Tan et al., 1987; Holdich and Lawson, 1987; Mgaidi et al., 1991; and Hagemann, 1999) and/or measured in this TP, will be used for determining the PIPs of a matrix ion-lead species (e.g., Na^{+}-$PbCl^{3-}$) and/or solubility constants of lead solids so that the WIPP relevant conditions are covered. PIPs will be determined in a process outlined in a forthcoming AP specific to this TP.

The work proposed in this document can be broken down into two basic phases: preparation of experiments and monitoring of experiments. The results of this study will provide an improved model for the solution thermodynamics of lead in the WIPP repository for CRA-2024.

3 EXPERIMENTAL PROCESS DESCRIPTION

Solid dissolution reactions and aqueous organic complex dissociation that have been identified in this test plan are listed in Table 1. The solids will either be purchased or synthesized and carefully characterized as appropriate to achieve a pure starting material (task 1). Synthesis of solids will be documented in the associated scientific notebooks per NP 20-2 “Scientific Notebooks”. Long-term solubility experiments will be performed for the solids identified for study in various conditions at undersaturation (task 2). Solubility constants will be determined for each solid in WIPP relevant

brines and experiments will be monitored over time to determine the solid formation products of the various systems. The process of calculating PIPs and solubility constants collected from this TP will be addressed in a separate forthcoming AP. A series of scoping experiments will be set up with additional variables such as composition of background solutions (task 3). A set of reactions that have been identified for study can be seen in Table 1. These reactions have been identified as possible formation products in literature studies and previous SNL work. (Nuclear Decommissioning Authority, 2016; Edwards et al., 1992; Olby, 1966; and Regenspurg et al., 2016).

Table 1.

Solid Dissolution Reactions, Organic Complex Dissociation Reactions, and Possible Lead - Organic Solids
$PbCl_2$ (cotunnite) ↔ $Pb^{2+} + 2Cl^-$
α-PbO (litharge) + $2H^+$ ↔ $Pb^{2+} + H_2O$
PbO (massicot) + $2H^+$ ↔ $Pb^{2+} + 2H_2O$
PbCl(OH) (laurionite) + H^+ ↔ $Pb^{2+} + H_2O + Cl^-$
$Pb_8O_5(OH)_2Cl_4$ (blixite) + $12H^+$ ↔ $8Pb^{2+} + 7H_2O + 4Cl^-$
$PbCO_3$ (cerussite) + H^+ ↔ $Pb^{2+} + HCO_3^-$
$Pb_3(CO_3)_2(OH)_2$ (hydrocerussite) + $4H^+$ ↔ $3Pb^{2+} + 2H_2O + 2HCO_3^-$
$NaPb_2(CO_3)_2(OH)$ (abellaite) + $3H^+$ ↔ $Na^+ + 2Pb^{2+} + H_2O + 2HCO_3^-$
$Pb_2CO_3Cl_2$(s) (phosgenite) + H^+ ↔ $2Pb^{2+} + HCO_3^- + 2Cl^-$
$Pb_{10}(CO_3)O_6(OH)_6$ (plumbonacrite) + $19H^+$ ↔ $10Pb^{2+} + HCO_3^- + 12H_2O$
$PbSO_4$ (anglesite) + H^+ ↔$Pb^{2+} + HSO_4^-$
$Pb(Oxalate)_2^{2-}$ ↔ $Pb^{2+} + 2Oxalate^{2-}$ and PbOxalate(aq) ↔ Pb^{2+} + $Oxalate^{2-}$
$Pb(Citrate)^-$ ↔ $Pb^{2+} + Citrate^{3-}$
$PbEDTA^{2-}$ ↔ $Pb^{2+} + EDTA^{4-}$
Lead Oxalate (s)
Lead Citrate (s)
Lead EDTA (s)

3.1 Task List

3.1.1 Task 1: Synthesize and Characterize Solid Starting Materials

The majority of the lead starting solids, e.g., PbO(s), $PbCl_2$(s), $PbCO_3$(s), $PbSO_4$(s), and PbOxalate(s), can be purchased from commercial vendors such as Fisher Scientific and Alfa Aesar. However, there may be cases where the solid cannot be purchased and must be synthesized. Synthesis procedures for numerous lead solids have been identified in the literature and will be used as guides for synthesis in this task (Edwards et al., 1992; Marani et al., 1995; Olby, 1966). All starting solutions used for synthesis will be made using commercially available salts of ACS

grade or better. Synthesis procedures will vary based on the solids being prepared. All synthesis procedures will be documented in the associated scientific notebooks. All starting materials (synthesized and purchased) will be characterized using XRD and SEM/EDS before initiation of experiments to assess purity levels. Additional instrumentation listed in section 3.6 may be used for further characterization if necessary. Table 2 lists all experimental work for task 1.

Table 2. Task 1

Task #	
1.1	Identify/synthesize a source of cotunnite and characterize
1.2	Identify/synthesize a source of litharge and characterize
1.3	Identify/synthesize a source of massicot and characterize
1.4	Identify/synthesize a source of laurionite and characterize
1.5	Identify/synthesize a source of blixite and characterize
1.6	Identify/synthesize a source of cerussite and characterize
1.7	Identify/synthesize a source of hydrocerussite and characterize
1.8	Identify/synthesize a source of abellaite and characterize
1.9	Identify/synthesize a source of phosgenite and characterize
1.10	Identify/synthesize a source of plumbonacrite and characterize
1.11	Identify/synthesize a source of anglesite and characterize
1.12	Identify/synthesize a source of PbOxalate and characterize
1.13	Identify/synthesize a source of PbCitrate and characterize
1.14	Identify/synthesize a source of PbEDTA and characterize

3.1.2 Task 2: Long-term Solubility Experiments

Experiments will be initiated from undersaturation conditions for all the systems listed in Table 4. These experiments will be prepared inside a glove box to ensure a controlled environment, with minimal CO_2 and oxygen. The glove box atmosphere will be primarily nitrogen gas, with less than 1 ppm oxygen. A set of samples will be created, with an individual vial for each sample collection. Brines will be prepared with de-gassed DI water and ACS grade or better salts from commercial vendors. Experiments will be prepared with an excess of the lead solid starting material and the solution of interest. The amount of solid for each system may vary slightly based on the various solubilities of the solid being used as the solubility controlling phase. The concentration of the matrix solution will be chosen to encompass the entire range of possibilities for a specific solution (i.e. NaCl matrix 0 to ~6.0 m (saturation)). pH of the system will be self-buffered by the constituents present in the system; no pH adjustment will be made for this task. Fifteen vials of each test matrix will be set up for each individual listed task. An example of the test matrix can be seen in Table 3 for task 2.1. This design will be implemented for all other sub-tasks in task 2 with their respective background matrices. Each vial prepared will be crimped in a glass serum vial and prepared and stored inside an atmosphere-controlled glove box. Each vial will be labeled 1 through 15 to ensure traceability and stored inside an atmosphere-controlled glovebox. When sampling occurs, the first vial in the series of 15 will be de-crimped, pH and solution temperature will be measured in-situ and then the entire vial will be terminated. The entirety of the solution will be collected and filtered using a 0.2 µm Acrodisc® nylon membrane syringe filter. The solid will be allowed to dry in the original vial, inside the glove box. Once dry and the filtrate has been removed,

the solid will be briefly washed with DI water or other appropriate solvent to remove the matrix, using vacuum filtration. Small amounts of solid of interest may be lost in this washing process, although losses will be minimal due to the low solubility of the solubility controlling solid and high solubility of the matrix solution. If solubility controlling solids are not washed, the lead solid spectrum is over-whelmed by the spectra of the matrix solution and usable data cannot be obtained using XRD. Solids and filtrate collected will be stored inside the glovebox until ready for analysis. Non-preserved filtrate (filtrate that is not diluted and does not contain acid) will remain inside the glovebox in a crimped serum vial, and only subsequent dilutions will be removed from the glove box for analysis. Analysis will be completed as soon as possible after sample collection. The sample collection date and time will be recorded in the scientific notebook for every sample collection, so the exact "age" of the sample will be known at the time of analysis. Filtrate will be discarded per SNL ES&H guidelines after analysis is complete. Exact timelines for stability of the liquid and solid phases for these experiments are not yet known, and because of that, SNL will conduct an independent study to determine solution and solid stability under the existing conditions, and will document the results in a memo to SNL WIPP records center. This will allow our program to develop a base-line for shelf-life of collected samples (filtrate, subsequent dilutions, and solid storage). Exact volumes of matrix solution and solid mass used will vary based on the different systems being tested. All experiments will be set up in duplicates. This solid to liquid ratio will be maintained for this task unless it is deemed that more solid will be needed for analysis or if dissolution of the solid occurs. In these cases, solid mass will be increased in the experiment.

Table 3. EXAMPLE Experimental Setup

Sample Name	Lead Solids, g	Solution Matrix, m	Solution Matrix mL/Vial	# of vials prepared
Sample 0-1	0.2-1.0	0	15-25	15
Sample 0-2	0.2-1.0	0	15-25	15
Sample 0.01-1	0.2-1.0	0.01	15-25	15
Sample 0.01-2	0.2-1.0	0.01	15-25	15
Sample 0.1-1	0.2-1.0	0.1	15-25	15
Sample 0.1-2	0.2-1.0	0.1	15-25	15
Sample 1.0-1	0.2-1.0	1	15-25	15
Sample 1.0-2	0.2-1.0	1	15-25	15
Sample 2.0-1	0.2-1.0	2	15-25	15
Sample 2.0-2	0.2-1.0	2	15-25	15
Sample 3.0-1	0.2-1.0	3	15-25	15
Sample 3.0-2	0.2-1.0	3	15-25	15
Sample 4.0-1	0.2-1.0	4	15-25	15
Sample 4.0-2	0.2-1.0	4	15-25	15
Sample 5.0-1	0.2-1.0	5	15-25	15
Sample 5.0-2	0.2-1.0	5	15-25	15
Sample 6.0-1	0.2-1.0	6	15-25	15
Sample 6.0-2	0.2-1.0	6	15-25	15

*0 m NaCl will consist of DI water.

Table 4. Task 2

Task #	Title
2.1	Cotunnite solubility in NaCl matrix (0.0 m-6.0 m)
2.2	Cotunnite solubility in $MgCl_2$ matrix (0.0 m-3.0 m)
2.3	Cotunnite solubility in mixed matrix (NaCl and $MgCl_2$)
2.4	Litharge solubility in NaCl matrix (0.0 m-6.0 m)
2.5	Litharge solubility in $MgCl_2$ matrix (0.0 m-3.0 m)
2.6	Litharge solubility in mixed matrix (NaCl and $MgCl_2$)
2.7	Massicot solubility in NaCl matrix (0.0 m-6.0 m)
2.8	Massicot solubility in $MgCl_2$ matrix (0.0 m-3.0 m)
2.9	Massicot solubility in mixed matrix (NaCl and $MgCl_2$)
2.10	Laurionite solubility in NaCl matrix (0.0 m-6.0 m)
2.11	Laurionite solubility in $MgCl_2$ matrix (0.0 m-3.0 m)
2.12	Laurionite solubility in mixed matrix (NaCl and $MgCl_2$)
2.13	Blixite solubility in NaCl matrix (0.0 m-6.0 m)
2.14	Blixite solubility in $MgCl_2$ matrix (0.0 m-3.0 m)
2.15	Blixite solubility in mixed matrix (NaCl and $MgCl_2$)
2.16	Cerussite solubility in NaCl matrix (0.0 m-6.0 m)
2.17	Cerussite solubility in $MgCl_2$ matrix (0.0 m-3.0 m)
2.18	Cerussite solubility in mixed matrix (NaCl and $MgCl_2$)
2.19	Hydrocerussite solubility in NaCl matrix (0.0 m-6.0 m)
2.20	Hydrocerussite solubility in $MgCl_2$ matrix (0.0 m-3.0 m)
2.21	Hydrocerussite solubility in mixed matrix (NaCl and $MgCl_2$)
2.22	Abellaite solubility in NaCl matrix (0.0 m-6.0 m)
2.23	Abellaite solubility in $MgCl_2$ matrix (0.0 m-3.0 m)
2.24	Abellaite solubility in mixed matrix (NaCl and $MgCl_2$)
2.25	Phosgenite solubility in NaCl matrix (0.0 m-6.0 m)
2.26	Phosgenite solubility in $MgCl_2$ matrix (0.0 m-3.0 m)
2.27	Phosgenite solubility in mixed matrix (NaCl and $MgCl_2$)
2.28	Plumbonacrite solubility in NaCl matrix (0.0 m-6.0 m)
2.29	Plumbonacrite solubility in $MgCl_2$ matrix (0.0 m-3.0 m)
2.30	Plumbonacrite solubility in mixed matrix (NaCl and $MgCl_2$)
2.31	Anglesite solubility in NaCl matrix (0.0 m-6.0 m)
2.32	Anglesite solubility in $MgCl_2$ matrix (0.0 m-3.0 m)
2.33	Anglesite solubility in mixed matrix (NaCl and $MgCl_2$)
2.34	Lead Oxalate solubility in NaCl matrix (0.0 m-6.0 m)
2.35	Lead Oxalate solubility in $MgCl_2$ matrix (0.0 m-3.0 m)
2.36	Lead Oxalate solubility in mixed matrix (NaCl and $MgCl_2$)
2.37	Lead Citrate solubility in NaCl matrix (0.0 m-6.0 m)
2.38	Lead Citrate solubility in $MgCl_2$ matrix (0.0 m-3.0 m)
2.39	Lead Citrate solubility in mixed matrix (NaCl and $MgCl_2$)
2.40	Lead EDTA solubility in NaCl matrix (0.0 m-6.0 m)

Task #	Title
2.41	Lead EDTA solubility in $MgCl_2$ matrix (0.0 m-3.0 m)
2.42	Lead EDTA solubility in mixed matrix (NaCl and $MgCl_2$)

3.1.3 Task 3: Scoping Experiments

The solubilities of cotunnite ($PbCl_2$(s)) and litharge (PbO(s)) in the brine of various composition will be measured in this task.

Each reactor will be investigated at least four times, i.e., at 1 week, 1 month, 2 months, and 3 months. During the investigations at 1 week, 1 month, and 2 months, the solution composition will be measured, such as, pH, concentrations of cations and anions. After the solution composition measurements at 3 months, the time-dependent measurement data will be compared to determine whether the reactors have reached equilibrium. The reactors determined to have reached equilibrium will be terminated to collect the final solids, and the final solids will be characterized by XRD. Further monthly investigations will be performed on the reactors determined not to have reached the equilibrium at the 3-month investigation. Table 5 lists all subtasks in task 3 and amount (volume or molality) of chemicals required for sample preparation.

Table 5. Task 3

Task #	To be prepared by end of August 2020			
3.1	Solubility of $PbCl_2$ in Water			
	Reactor ID	$PbCl_2$, g	NA [A]	Water, mL
	PbCl2DI-1	3.0	NA	50
	PbCl2DI-2	3.0	NA	50
	PbCl2DI-3	3.0	NA	50
3.2	Solubility of $PbCl_2$ in HCl solutions			
	Reactor ID	$PbCl_2$, g	HCl, m	Volume, mL
	PbCl2HCl-1-1	3.0	0.1	50
	PbCl2HCl-1-2	3.0	0.1	50
	PbCl2HCl-2-1	3.0	1.0	50
	PbCl2HCl-2-2	3.0	1.0	50
	PbCl2HCl-3-1	3.0	2.3	50
	PbCl2HCl-3-2	3.0	2.3	50
	PbCl2HCl-4-1	3.0	3.6	50
	PbCl2HCl-4-2	3.0	3.6	50
	PbCl2HCl-5-1	3.0	4.9	50
	PbCl2HCl-5-2	3.0	4.9	50
	PbCl2HCl-6-1	3.0	6.5	50
	PbCl2HCl-6-2	3.0	6.5	50
3.3	Solubility of $PbCl_2$ in NaCl solutions			
	Reactor ID	$PbCl_2$, g	NaCl, m (loading*)	Water, mL
	PbCl2NaCl-1-1	3.0	0.1	50
	PbCl2NaCl-1-2	3.0	0.1	50
	PbCl2NaCl-2-1	3.0	0.5	50
	PbCl2NaCl-2-2	3.0	0.5	50
	PbCl2NaCl-3-1	3.0	1.0	50
	PbCl2NaCl-3-2	3.0	1.0	50
	PbCl2NaCl-4-1	3.0	1.5	50
	PbCl2NaCl-4-2	3.0	1.5	50
	PbCl2NaCl-5-1	3.0	2.3	50

Task #	To be prepared by end of August 2020				
	PbCl2NaCl-5-2	3.0	2.3	50	
	PbCl2NaCl-6-1	3.0	3.6	50	
	PbCl2NaCl-6-2	3.0	3.6	50	
	PbCl2NaCl-7-1	3.0	4.9	50	
	PbCl2NaCl-7-2	3.0	4.9	50	
	PbCl2NaCl-8-1	3.0	6.5	50	
	PbCl2NaCl-8-2	3.0	6.5	50	
3.4	Solubility of $PbCl_2$ in NaOH: Scan for secondary lead minerals				
	Reactor ID	$PbCl_2$, g	NaOH, m	Water, mL	
	PbCl2NaOH-1-1	3.0	0.05	50	
	PbCl2NaOH-1-2	3.0	0.05	50	
	PbCl2NaOH-2-1	3.0	0.1	50	
	PbCl2NaOH-2-2	3.0	0.1	50	
	PbCl2NaOH-3-1	3.0	0.2	50	
	PbCl2NaOH-3-2	3.0	0.2	50	
	PbCl2NaOH-4-1	3.0	0.3	50	
	PbCl2NaOH-4-2	3.0	0.3	50	
	PbCl2NaOH-5-1	3.0	0.5	50	
	PbCl2NaOH-5-2	3.0	0.5	50	
	PbCl2NaOH-6-1	3.0	1.0	50	
	PbCl2NaOH-6-2	3.0	1.0	50	
3.5	Solubility of $PbCl_2$ in $MgCl_2$ solution				
	Reactor ID	$PbCl_2$, g	$MgCl_2$, m (loading*)	Water, mL	
	PbCl2MgCl2-1-1	3.0	0.1	50	
	PbCl2MgCl2-1-2	3.0	0.1	50	
	PbCl2MgCl2-2-1	3.0	0.5	50	
	PbCl2MgCl2-2-2	3.0	0.5	50	
	PbCl2MgCl2-3-1	3.0	1.5	50	
	PbCl2MgCl2-3-2	3.0	1.5	50	
	PbCl2MgCl2-4-1	3.0	2.0	50	
	PbCl2MgCl2-4-2	3.0	2.0	50	
	PbCl2MgCl2-5-1	3.0	2.5	50	
	PbCl2MgCl2-5-2	3.0	2.5	50	
	PbCl2MgCl2-6-1	3.0	3.0	50	
	PbCl2MgCl2-6-2	3.0	3.0	50	
3.6	Solubility of PbO in Na_2H_2EDTA solutions				
	Reactor ID	PbO, g	Na_2H_2EDTA, m	$Mg(OH)_2$, g	Water, mL
	PbONa2H2EDTA-1-1	6.0	0.01	0.0	50
	PbONa2H2EDTA-1-2	6.0	0.01	1.0	50
	PbONa2H2EDTA-2-1	6.0	0.03	0.0	50
	PbONa2H2EDTA-2-2	6.0	0.03	1.0	50
	PbONa2H2EDTA-3-1	6.0	0.06	0.0	50
	PbONa2H2EDTA-3-2	6.0	0.06	1.0	50
	PbONa2H2EDTA-4-1	6.0	0.10	0.0	50
	PbONa2H2EDTA-4-2	6.0	0.10	1.0	50
	PbONa2H2EDTA-5-1	6.0	0.15	0.0	50
	PbONa2H2EDTA-5-2	6.0	0.15	1.0	50
	PbONa2H2EDTA-6-1	6.0	0.20	0.0	50
	PbONa2H2EDTA-6-2	6.0	0.20	1.0	50

[A] Not Applicable, * Loading is a term that can be used to indicate the salt is added over its solubility limit.

3.2 Overall Strategy and Process

The overall strategy of this test plan is to determine the solubility constants and solid formation products and rates of solid formation in various lead systems relevant to WIPP.

- Critical Variables to be Measured:

  pH: measured and controlled utilizing the procedures and acceptance criteria outlined in SP 12-14, "Use of pH meters and Electrodes". A pH electrode that is recommended for high ionic strengths will be used for pH measurement. If warranted, a pH correction factor will be applied to these measurements at different ionic strengths in specific brines as measured in TP 18-01 (Kirkes, 2019) or this study.

  Temperature: Temperature will be measured using a calibrated temperature probe per SP 12-20 "Thermometer Calibration Check". Temperature will be measured on sample solution for each vial and time samples are collected. Solution temperatures will be recorded in the scientific notebooks.

  Starting Solution Analysis: All solutions to be used as matrices will be prepared using solids certified as ACS grade or better. Densities will be measured of each solution after preparation and documented in a scientific notebook. Densities will be measured volumetrically (utilizing tared Class A glassware and recording the weight; (ASTM E288-10(2017), ASTM E1272-02(2019)) or estimated using established literature sources such as, Sőhnel and Novotný (1985). All constituents in the solutions will be verified for expected concentrations using instrumentation such as the ICP-AES, ICP-MS, IC and other means as deemed necessary. Complex brines will be prepared in accordance with SP 20-4, "Preparing Synthetic Brines for Geochemical Experiments". All solution preparation and analysis will be documented in a scientific notebook. Criteria documented in the Specific Procedures (SPs) will be used to determine data acceptance for these analyses.

  Sample Solution Analysis: All sample solutions will be analyzed for all relevant dissolved components at each sampling cycle for task 2 and as relevant for task 3. The initial dilution for solution chemistry analysis will be done using a gravimetric technique. i.e. if a 10X dilution is needed, a scale will be tarred with a 10 mL volumetric flask then ~1 g of sample will be added. Subsequent dilutions can be made using a pipette or volumetric flasks. The final measured concentration will be corrected by using the exact by weight dilution and density corrected value. All constituents in the solutions will be verified for expected concentrations using instrumentation such as the ICP-AES, ICP-MS, IC, Carbon Coulometer and other means as deemed necessary. Complex brines will be prepared in accordance with SP 20-4. All solution preparation and analysis will be documented in a scientific notebook. Criteria documented in the SPs will be used to determine data acceptance for these analyses.

  Sample Solid Analysis: All starting solids will be characterized using XRD and SEM/EDS. Other techniques may be employed such as BET surface analysis, TGA/DSC and Raman spectrometry if necessary. For task 2 solids will be characterized at each sampling. For task 3 solids will be characterized as appropriate for the specific test.

- Coordination with other Organizations: All activities associated with this test plan will be monitored and performed within the SNL CPG organizations. Interaction with other SNL organizations may occur on a case by case basis (i.e. technical reviews).

- A variety of M&TE will be used for the work described in this TP. A complete list of this M&TE, including serial numbers, will be established and maintained in the scientific notebooks. The user(s) of all the equipment specified in section 3.6.4 will follow the appropriate SP and/or user's manual for each instrument.

- Error and Uncertainty: Potential sources of error in this TP can be contributed by items such as; pH measurement, volume measurement, weighing errors, impure reagents, temperature, variation in sample preparation, variation in dilution preparation, instrumentation error and improper set-up or control of experiment.

Weight measurements, and the control of the sample during processing will be conducted in accordance with SP 12-1 "Use of Laboratory Balances and Scales" and NP 13-1 "Control of Samples and Standards". The respective acceptance criteria and uncertainties for these measurements are discussed in those documents.

Volume measurement errors will be controlled by utilizing only Class A glassware for all solution preparation and calibrated pipettes. Pipettes will be calibrated prior to use and the calibration shall be documented in the associated scientific notebooks.

Impure reagent errors will be controlled by using only solids certified as ACS grade or better for solution preparation. In addition, all solutions will be characterized using elemental analysis techniques after preparation to confirm desired purity and concentration.

Variation in sample preparation could cause issues with data comparisons between similar experimental set-ups. To account for this all experiments will be set up in duplicate and all experimental parameters for set up will be recorded in associated scientific notebooks so discovered anomalies can be pinpointed. Additionally, samples will be measured up to 15 times to ensure repeatability in collected results.

Temperature error will be controlled by measuring the temperature of the solution being sampled, therefore temperature effects can be considered in anomalous data. The thermometer used for the temperature measurement will be a calibrated or calibration checked thermometer per SP 12-20 "Thermometer Calibration Check".

Instrumentation error will be controlled by the various activity specific procedures for each instrument. The acceptance criteria for each instrument is outlined in the respective procedures.

- Data Processing: Data processing will be accomplished using the software provided with each instrument, in addition to off-the-shelf software such as Microsoft Excel. If Microsoft Excel or other software's are used to complete calculations, the calculations will be reviewed along with the scientific notebooks and milestone reporting.

- Laboratory activities will be recorded in scientific notebooks, and they will be maintained as quality assurance (QA) records.

3.3 Sample Control

The sample control for the work under this test plan will follow the WIPP procedure NP 13-1, "Control of Samples and Standards". Each sample will be appropriately labeled with a unique sample ID and the date of preparation. Sample preparation and utilization will be documented in scientific notebooks.

All long-term solubility experiments will be prepared and stored in an atmospherically controlled glove box with oxygen values below 5 ppm. Nitrogen will be used as the atmosphere gas in the glove box environment. For task 2 each individual vial will additionally be crimp sealed in a glass serum vial and it will not be disturbed until ready to be terminated. When samples are terminated or disposed, the action will be recorded in the associated scientific notebooks to ensure traceability.

3.4 Data Quality Control

3.4.1 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 procedure 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.

3.4.2 Data Acquisition System

Data collection procedures are specific to individual instruments. For details of the data acquisition for an instrument, see the SP or user's manual for that instrument. Any data acquired by a data acquisition system (DAS) will be attached directly to the scientific notebooks or compiled in separate loose-leaf binders with identifying labels to allow cross reference to the appropriate scientific notebooks. If the instrument allows data to be recorded electronically, copies of the data disks will be submitted to the SNL WIPP Records Center according to procedure NP 17-1, "Records". If possible, data files may be transferred to portable data storage devices or a 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 notebooks.

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.

Commercial Software List	
Operating Software/Database	Instrument
Syngistix Version 3.0.4.3510	ICP-AES
Syngistix Version 2.4	ICP-MS
UIC Carbon Coulometer 3.7	Carbon Coulometer
Chromeleon Version 7.2.8	IC
Microsoft Excel	SNL-owned computers
STA 409 and Proteus Commission number: 206.011.412/05 Software order: SW/STA/675.288 SW/STA/675.244	TGA/DSC
JSM-5000 5.52	SEM
NSS 2.3	EDS
ASAP2020 4.03	ASAP 2020
LabSpec6/KnowItAll database 2014 6.1.7601	Raman Spectrometer
Cary WinUV 5.1	UV-Vis
Diffrac.SUITE, Diffrac.EVA/PDF4+ database 7.5.0	XRD

All instrument reference samples and other control samples will be prepared and controlled in accordance with the SPs associated with the instruments.

3.5 Data Identification and Use

All calculations and data generated as part of the activities of this TP 20-01 will be documented in a scientific notebook. The notebook will be reviewed periodically to ensure that the technical and QA requirements of procedure NP 20-2, “Scientific Notebooks”, are met. If a discrepancy is found, that discrepancy and its resolution will be documented during the review on a Document Review and Comment (DRC) Form NP 6-1-1.

3.6 Equipment and Techniques

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 notebooks. Scientific notebooks will be used to record all laboratory work activities.

3.6.1 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 NIST-traceable weight sets, which, in turn, are calibrated by the SNL Primary Standards Laboratory. Calibration checks will be recorded in a Balance Calibration Records log book. Balance usage will follow SP 12-1.

3.6.2 Liquid Measuring Equipment

Standard Laboratory Class A glassware (glass pipettes, volumetric flasks, etc.) and adjustable pipettes will be used for all measurements involving liquids. The calibration of adjustable pipettes will be checked prior to use against a calibrated balance and will be recorded in the scientific notebooks. The accuracy of the pipettes will be within 1% of the expected value.

3.6.3 Temperature Control Equipment

Thermal bath(s) with circulation will be acquired to provide a better temperature control for experiments in task 3. The thermal bath has cooling/heating units and can circulate the media to a vessel so that all experiments are controlled at a desirable temperature with a small fluctuation.

3.6.4 Other Analytical Equipment & Techniques

A. Temperature Measuring Equipment-Temperature will be measured using a calibrated thermometer. Temperature measurements will be collected on the solutions being collected/tested.

B. pH Meters and Autotitrators – Solution pH will be measured using pH meters or a pH probe autotitrator assembly. The pH probes and meters used will be recorded in the appropriate scientific notebooks at the time of use. The range for all pH meters is 0.00 to 14.00. SP 12-14 will be followed for this procedure.

C. Equipment for Chemical Analysis– The following instruments may be used for chemical analyses:

- Balances
- Carbon Coulometer
- XRD
- ICP-AES
- Particle Sizer (Mastersizer)
- TGA/DSC
- SEM/EDS
- IC
- UV-Vis Spectrophotometer
- ICP-MS
- ASAP 2020
- Refractometer
- Raman Spectrometer

The usage of these instruments will follow the respective SPs.

3.7 Records

Records shall be maintained as described in this TP and applicable QA implementing procedures (NPs and SPs). These records may consist of bound scientific notebooks, loose-leaf pages, forms,

printouts, or information stored on electronic media. The PI will ensure that the required records are maintained and are submitted to the SNL WIPP Records Center according to NP 17-1, "Records".

3.7.1 Required QA Records

At a minimum, QA records will include:

- Scientific notebooks;
- NPs and SPs used;
- Calibration records for controlled equipment and/or equipment specification or information sheets supplied by the manufacturer.

3.7.2 Miscellaneous Non-QA Records

Additional records that are useful in documenting the history of the activities but are considered non-QA Records per the definition outlined in the NP Glossary, may be maintained and submitted to the SNL WIPP Records Center. These records include:

- Equipment manuals and specifications;
- photographs taken by member of workforce (MOW) during experiments, or to document experimental results
- electronic media collected from instrumentation for better resolution (i.e. electronic media from SEM, XRD)

These records do not support performance assessment or regulatory compliance and, therefore are not quality-affecting information.

4 TRAINING

All personnel involved in the experiments described in this test plan will be trained and qualified for their assigned work. This requirement will be implemented through procedure NP 2-1, "Qualification and Training". Specifically, the following NPs and SPs are applicable:

- NP 2-1– "Qualification and Training"
- NP 6-1– "Document Review Process"
- NP 12-1– "Control of Measuring and Test Equipment"
- NP 13-1– "Control of Samples and Standards"
- SP 13-1– "Chain of Custody"
- NP 17-1– "Records"
- NP 20-2 – "Scientific Notebooks"

5 HEALTH AND SAFETY

All the health and safety requirements relevant to the activity level work described in this TP and the procedures that will be used to satisfy these requirements are described in SNL ES&H Manual (MN471022) (weblink is in reference section).

6 PERMITTING/LICENSING

There are no special license or permit requirements for the activities described in this test plan.

7 REFERENCES

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