Sandia National Laboratories
Waste Isolation Pilot Plant

Prediction of Baseline Actinide Solubilities for the 2026 WIPP Compliance Recertification Application Performance Assessment Interim-State Analysis (CRA-2026 IS)

Work Carried Out under Task 3 of the Analysis Plan for WIPP Near-Field Geochemical Process Modeling, AP 153, Rev. 1.
To be included in the AP-153 records package

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1 INTRODUCTION

The Waste Isolation Pilot plant (WIPP) was initially certified as a 10-panel repository for long-term waste disposal for transuranic (TRU) waste, which served as the design layout and basis for the performance assessment (PA) calculations for the 2019 Compliance Recertification Application Deferred Performance Assessment (CRA-2019 DPA). Due to operational constraints, not all this volume is available for waste disposal. In March 2024 the U.S. Department of Energy (DOE) submitted the Replacement Panels Planned Change Request (RPPCR) seeking U.S. Environmental Protection Agency (EPA) approval of two replacement waste disposal panels. Although the RPPCR is expected to be approved prior to submittal of 2026 Compliance Recertification Application (CRA-2026), the replacement panels will not accommodate the entire allowable waste volume as specified in the WIPP Land Withdrawal Act (LWA), leading to the consideration of seven additional waste panels. Thus, the CRA-2026 performance assessment (PA) will consider two repository designs: 1) An interim state repository (CRA-2026 IS) with 12 panels; and 2) a final-state repository[1] (CRA-2026 FS) with 19 panels, which provides sufficient storage for disposal of the entire WIPP LWA waste volume.

This report documents the baseline actinide solubility calculations the results of which will be included in the PA calculations for CRA-2026 IS, or the interim state. A separate report (Domski, 2025a) documents the baseline actinide solubility calculations for the PA calculations for the CRA-2026 FS.

This analysis report provides the new baseline solubilities of Th(IV), Np(V), and Am(III) in two standard Waste Isolation Pilot Plant (WIPP) brines as a function of the volumes of these brines in the repository for the CRA-2026 IS, and uses the WIPP thermodynamic database DATA0.FM6 (Domski, 2023c).

The CRA-2026 IS baseline solubility investigates the effect on actinide solubilities of decreasing the direct brine release (DBR) volume used in the RPPCR from 33,804 m^3 (King, 2021) to 6,314 m^3 (Brunell, 2025). This nearly 5.4x decrease in the DBR volume is attributed to new predictions of the porosity as the surrounding salt encroaches on and compresses the waste over time (Docherty, 2024, Brunell, 2025). The decreased DBR volume used for CRA-2026 IS had the effect of increasing the concentrations of the organic ligands (Domski, 2025b) used in the baseline solubility calculations.

Actinide solubilities (the sums of the concentrations of all dissolved actinide species in chemical equilibrium with actinide-bearing solid phases under the conditions expected in WIPP disposal rooms) and the concentrations of colloidal (suspended) actinides (calculated from the baseline solubilities) together constitute the actinide source term used in WIPP performance assessment (PA) calculations. These solubilities are often referred to as the "baseline solubilities" because they comprise unique values predicted using thermodynamic models for each actinide analog element and WIPP brine under expected near-field chemical conditions. The PA codes use the actinide solubilities, and a sampled uncertainty multiplier that describes possible deviations of the predicted baseline Th(IV) and Am(III) solubilities from experimentally measured solubilities. The

[1] For the remainder of the document when the "repository" is discussed it is the interim state repository unless otherwise specified.

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reason for using these uncertainty factors is to account for uncertainties in the model and parameters that comprise the thermodynamic database. The uncertainty factor distributions are calculated and documented in a separate analysis (Domski, 2025c).

The two standard WIPP brines used in these analyses are Generic Weep Brine (GWB) and Energy Research and Development Administration (WIPP Well) 6 (ERDA-6). GWB is a synthetic brine representative of intergranular Salado Formation (Fm.) brines at or near the stratigraphic horizon of the repository (Krumhansl et al., 1991; Snider, 2003). ERDA-6 (Popielak et al., 1983) is a synthetic brine representative of fluids in brine reservoirs in the Castile Fm., which underlies the Salado Fm.

Uranium(VI) solubility is not calculated in this baseline solubility model. The analysis does not provide any solubilities for U(VI) because a thermodynamic speciation-and-solubility model has not been implemented in the WIPP thermodynamic database. Rather, the EPA (U.S. EPA, 2006) has specified that a value of 1E-03 M be used in PA calculations for the solubility of U(VI) in GWB and ERDA-6. This value has been used since the CRA-2004 PABC, however, for the CRA-2026 IS Los Alamos National Laboratory (LANL) has issued a new U(VI) solubility value of 3.0E-06 M (Kaplan et al., 2025).

This analysis report also provides the chemical compositions of the reacted brines, and the values of parameters such as ionic strength, activity of water, f_{CO_2}, pH, pcH, and Total Inorganic Carbon (TIC). These intensive properties provide important data regarding the state of the system. These data for the CRA-2026 IS are tabulated in the following sections.

The CRA-2026 IS baseline solubility model differs from the RPPCR and CRA-2026 FS baseline solubility model (Domski, 2023a and 2025a, respectively) in two ways: 1) The CRA-2026 IS is based on a new DBR volume (Brunell, 2025) which affects the scaling of the reactants used in the solubility model; and 2) a new inventory was issued for CRA-2026 IS (Van Soest, 2025b) which provides updated inventories for the organic ligands and reactants used in the solubility model.

The interim and final state CRA-2026 baseline solubility models do not include the effects of cementitious materials on solubility of the +III, +IV, or +V actinides. However, analyses of these effects are provided in Appendix A.

Assumptions employed in the CRA-2019 DPA that were changed for the RPPCR and CRA-2026 FS baseline solubility models were carried over to CRA-2026 IS. The assumptions are summarized in Section 2.2.

Note, this analysis was performed using the same process described as used through the submission of CRA-2026 FS (Domski, 2025a), and therefore is a deviation from AP-153, Revision 1 (Brush et al., 2012). This analysis report, as per NP 9-1 (Nielsen, 2024), is considered a compliance decision analysis.

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Table 1 defines the abbreviations, acronyms, and initialisms used in this report.

Table 1. Abbreviations, Acronyms, and Initialisms.

Abbreviation, Acronym, or Initialism	Definition
Ac, acetate	CH_3COO^- or $CH_3CO_2^-$
Am, Am(III)	americium, americium in the +III oxidation state
Am	amorphous
anhydrite	$CaSO_4$
AP	analysis plan
Aq	aqueous
aragonite	$CaCO_3$,a polymorph of $CaCO_3$ that is metastable with respect to calcite
Atm	atmosphere(s)
B, B(III)	boron, boron in the +III oxidation state
Br, Br(−I)	bromine, bromine in the −I oxidation state
Brucite	$Mg(OH)_2$
C	carbon
Ca, Ca(II), Ca^{2+}	calcium, calcium in the +II oxidation state, calcium ion
Calcite	$CaCO_3$, the thermodynamically stable polymorph of $CaCO_3$
Cerussite	$PbCO_3$
Cit, citrate	$(CH_2COO)_2C(OH)(COO)^{3-}$ or $(CH_2CO_2)_2C(OH)(CO_2)^{3-}$
Cl, Cl(−I), Cl^-	chlorine, chlorine in the −I oxidation state, chloride ion
CMS	(Sandia/WIPP software) Configuration Management System
CO_2	carbon dioxide
CO_3^{2-}	carbonate
CPR	Cellulose, plastic and rubber
DB	(thermodynamic) database
CRA-2004	the first WIPP Compliance Recertification Application, submitted to the EPA in March 2004
CRA-2009	the second WIPP Compliance Recertification Application, submitted to the EPA in March 2009
CRA-2014	the third WIPP Compliance Recertification Application, submitted to the EPA in March 2014

Table 1 continued on next page

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Table 1. Abbreviations, Acronyms, and Initialisms (continued).

Abbreviation, Acronym, or Initialism	Definition
CRA-2019 DPA	The fourth WIPP Compliance Recertification Application, Deferred Performance Assessment submitted to the EPA in March 2019
RPPA-2022	Replacement Panels Performance Assessment
DBR	direct brine release
dolomite	$CaMg(CO_3)_2$, a carbonate mineral that nucleates and grows slowly under low-temperature conditions and is often suppressed (prevented from forming) in geochemical modeling calculations
DRZ	disturbed rock zone
EDTA	ethylenediaminetetraacetate, $(CH_2COO)_2N(CH_2)_2N(CH_2COO)_2)^{4-}$ or $(CH_2CO_2)_2N(CH_2)_2N(CH_2CO_2)^{4-}$
EPA	(U.S.) Environmental Protection Agency
EQ3/6	a geochemical software package for speciation and solubility calculations (EQ3NR) and reaction-path calculations (EQ6)
earlandite	$Ca_3[C_3H_5O(COO)_3]_2 \cdot 4H_2O$
ERDA-6	Energy Research and Development Administration (WIPP Well) 6, a synthetic brine representative of fluids in Castile brine reservoirs
f_{CO_2}	fugacity (similar to the partial pressure) of CO_2
Fm.	Formation
GWB	Generic Weep Brine, a synthetic brine representative of intergranular Salado brines at or near the stratigraphic horizon of the repository
Gypsum	$CaSO_4 \cdot 2H_2O$
H or H_2, H^+	hydrogen or hydrogen ion
Halite	NaCl
H_2O	water (aq, g, or contained in solid phases)
hydromagnesite	$Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$
I	ionic strength, defined by $I = ½ \times \Sigma_i(M_i \times z_i^2)$, in which M_i and z_i are the molarity and charge of species i
I/O	input/output
K, K(I)	potassium, potassium in the +I oxidation state
Kg	kilogram(s)
litharge	PbO
M	Molar, $mol \cdot dm^{-3}$

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Table 1. Abbreviations, Acronyms, and Initialisms (continued).

Abbreviation, Acronym, or Initialism	Definition
m	meters or molal, $mol \cdot kg^{-1}$
magnesite	$MgCO_3$
Mg, Mg(II)	magnesium, magnesium in the +II oxidation state
MgO	magnesium oxide, used to refer to the WIPP engineered barrier, which includes periclase as the primary constituent and various impurities
mM	millimolar
$Mg_3Cl(OH)_5 \cdot 4H_2O$	Magnesium chloride hydroxide tetrahydrate, phase 5
Na, Na(I), Na^+	sodium, sodium in the +I oxidation state, sodium ion
nesquehonite	$MgCO_3 \cdot 3H_2O$
Np, Np(V)	neptunium, neptunium in the +V oxidation state
O or O_2	oxygen
OH, OH^-	hydroxide or hydroxide ion
Ox, oxalate	$(COO)_2^{2-}$ or $C_2O_4^{2-}$
PA	performance assessment
PABC	Performance Assessment Baseline Calculations
Pb, Pb(II)	Lead, lead in the +II oxidation state
periclase	pure, crystalline MgO, the primary constituent of the WIPP engineered barrier
pH	the negative, common logarithm of the activity of H^+
pcH	the negative, common logarithm of the molar concentration of H^+
polyhalite	$K_2MgCa_2(SO_4)_4 \cdot 2H_2O$
QA	quality assurance
Rev.	revision
RH	relative humidity
S, S(VI), SO_4^{2-}	sulfur, sulfur in the +VI oxidation state, sulfate ion
SCA	S. Cohen and Associates
SNL	Sandia National Laboratories
Th, Th(IV)	thorium, thorium in the +IV oxidation state
TIC	total inorganic C
U, U(IV), U(VI)	uranium, uranium in the +IV oxidation state, uranium in the +VI oxidation state
whewellite	$CaC_2O_4 \cdot H_2O$
WIPP	Waste Isolation Pilot Plant
wt %	weight percent

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2 METHODS

The objective of this analysis is to provide the solubilities of the actinide elements Am(III), Th(IV), and Np(V), in the standard WIPP brines GWB and ERDA-6 in contact with the geologic environment, the engineered barrier materials, and the waste package materials as a function of the volume of these brines in the repository. Brush et al. (2012) described the methods used to calculate the solubilities Am(III), Th(IV), and Np(V) for use in WIPP PA, why the brines GWB and ERDA-6 are used, how these solubilities are applied to other actinides included in WIPP PA, etc. The methods that we used for this analysis were identical to those used by Domski and Sisk-Scott (2019) for the CRA-2019 DPA, the RPPCR (Domski, 2023a), and the CRA-2026 FS (Domski, 2025a).

We used EQ3/6, Version 8.0a (Wolery and Jarek, 2003; Wolery, 2008; Wolery et al., 2010, and Wolery, 2013) to simulate the reaction of GWB and ERDA-6 with the important solids in the WIPP. In the first step of this reaction (referred to herein as "Step 1"), we added the following compounds to GWB and ERDA-6 using EQ3NR: (1) Acetate, citrate, EDTA, and oxalate; and (2) ThO_2(am), $KNpO_2CO_3$, and $Am(OH)_3$(am)), the solids most likely to control the solubilities of Th(IV), Am(III), and Np(V) in the repository (Brush et al., 2012). In Step 2, using EQ6, these brines were reacted with the important solids in the repository (see below) in a manner consistent with the conceptual models for WIPP near-field chemistry (SCA, 2008; Brush et al., 2012).

As a reaction-path code EQ6 runs until either of the following conditions are met: 1) All of the reactants are consumed – a potential non-equilibrium scenario; or 2) until the solution is in equilibrium with both the remaining reactant phases and with the product phases. For the WIPP baseline solubility calculations the second case applies, the final, or equilibrium reacted brine compositions are in equilibrium with both the reactant phases and any product phase which formed during the reaction. After equilibration, the compositions of these brines define so-called invariant points (one each for GWB and ERDA-6), because the solids specified in the conceptual models — in particular brucite ($Mg(OH)_2$) and hydromagnesite ($Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$) — control the new compositions of the brines and parameters such as fCO_2, pH, pcH, TIC.

2.1 Model Setup

Calculation of the actinide baseline solubilities follows a two-step process:

Step 1: Calculation of Initial Solution Compositions with EQ3NR

- EQ3NR is used to equilibrate and speciate the brine compositions (ERDA-6 & GWB) with the inventory scaled masses of the organic ligands (acetate, oxalate, citrate, and EDTA).
- The actinide concentrations of the initial solutions are set via equilibrium with solubility controlling phases ($Am(OH)_3$(am), ThO_2(am), and $KNpO_2CO_3$).
- The conditions of relatively low pH and high carbonate concentration (Table 3 below) of the initial solution ensures that an excess mass of actinides dissolve in this step.
- The initial solution composition(s), which includes the dissolved actinide concentrations are then passed to Step 2 via the EQ3NR pick up file and are reacted with the solids and subject to the evolving chemical environment where the stable actinide solubility controlling phases may form.

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Step 2: Calculation of Equilibrium Solution Compositions with EQ6

- Using EQ6, the initial solution compositions from Step 1 are reacted with:
  - Inventory-scaled masses of the MgO barrier (50% brucite and 50% hydromagnesite)
  - Iron and lead reactants representing the waste containers and radiation shielding
  - Salado Formation minerals halite and anhydrite
- The model includes the effects of organic ligand complexation and mineral phase dissolution and precipitation.
- The model provides the actinide solubilities and the near-field chemistry including:
  - Equilibrium pH
  - Carbon dioxide fugacity
  - Activity of water
  - Total inorganic carbon
  - Ionic strength
  - Concentration of all dissolved constituents
  - Solid phase (reactant and product phase) budget

As outlined above the EQ3/6 baseline solubility runs are completed in two steps. For Step 1, the speciation and solubility code EQ3NR was used to "solve the initial solutions", in other words the code reads the input files containing the data discussed above, and speciates the solution, dissolves the solubility-controlling actinide phases in the presence of organics, and calculates the mineral saturation index values for GWB and ERDA-6. The low pH and high carbonate concentrations of the initial brine compositions ensures that an excess amount of the solubility-controlling actinide phases dissolve in the brines during Step 1.

There are five input files for each brine each representing a different brine volume, the only input that changes are the organic ligand concentrations. EQ3NR code outputs two ascii files, a user friendly output file (*.3o) which is useful to the analyst as it provides solution speciation data, mineral saturation information, and other intensive solution properties, and a second file, the pickup file (*.3p) which contains the same information but in a format that is used by EQ6 to setup the initial conditions of the reaction path run.

For Step 2, the reaction-path code EQ6 was used to titrate (incrementally add) the reactants halite, anhydrite, brucite, hydromagnesite, hibbingite and hydrocerussite into GWB and ERDA-6 resultant solutions from Step 1. Halite and anhydrite were used to simulate the most important minerals[2] in the Salado Fm. at or near the stratigraphic horizon scaled to their masses in the disturbed-rock zone (DRZ) of the repository; and brucite and hydromagnesite to simulate the expected hydration and carbonation products, respectively, of MgO (the WIPP engineered barrier), hydrocerussite to represent the corroded lead product when lead shielding in the waste packages is corroded under anoxic conditions, the corroded waste drum and waste iron materials are represented by hibbingite ($Fe_2Cl(OH)_3$). The EQ6 input values for each reactant are tabulated in

[2] During the CRA-2019 DPA completeness evaluation the EPA requested that a sensitivity study be performed which included polyhalite as a reactant, the results showed it had negligible effect on actinide solubility (Knerr, 2021).

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Table 5. The input reactant moles (Table 5) were scaled down from the repository scale data presented in the Performance Assessment Inventory Report (PAIR) 2024 (Van Soest, 2025b) to values consistent with the 1 Kg brine volume of EQ3/6.

EQ6 was used in closed-system mode (model variable IOPT1 = 0) for Step 2. Closed-system mode consists of the simulated titration (incremental addition) of the reactants described above to GWB or ERDA-6. "Closed-system" means that no reactants or products can leave the system after the reactants are titrated in, which simulates the WIPP under undisturbed conditions. Mineral phases that were suppressed for the CRA-2026 IS (prevented from precipitating) included Calcite ($CaCO_3$), dolomite ($CaMg(CO_3)_2$), magnesite ($MgCO_3$), nesquehonite ($MgCO_3 \cdot 3H_2O$), hydromagnesite with the composition $Mg_4(CO_3)_3(OH)_2 \cdot 3H_2O$, phase 5 ($Mg_3Cl(OH)_5.4H_2O$), and $Am(OH)_3(s)$. Also suppressed was the aqueous species $FeEDTA^{2-}$ throughout Step 2. The rationale for suppressing these phases is discussed in Brush et al. (2012) and Domski (2023a).

Note, the EQ3/6 simulations are performed in two steps which implies there may be a temporal dependance on the order which the solid materials are contacted by the GWB or the ERDA-6 brines. This is not the case. All of the important solid materials are contacted with the brines simultaneously; this supports the conceptual model assumption of chemical homogeneity and solubility equilibrium and allows for the assumption of instantaneous reactions (Wilson et al., 1996).

For CRA-2026 IS the same model assumptions first implemented for the RPPCR (Domski, 2023a) were again implemented: 1) Calcite was suppressed and aragonite allowed to form; 2) the aqueous species $FeEDTA^{2-}$ was suppressed; 3) $FeCitrate^{-}$ and $FeOHCitrate^{2-}$ aqueous species were allowed in the CRA-2026 IS baseline solubility calculations; 4) $Am(OH)_3(am)$ will be used as the solubility controlling phase in Step 1, and $Am(OH)_3(s)$ was suppressed in Step 2; and 5) the iron and lead reactants were hibbingite and hydrocerussite, respectively. For discussions of these assumptions see Domski (2023a).

For CRA-2026, in both Steps 1 and 2, the DATA0.FM6 thermodynamic database as documented in Domski (2023c) was used for all EQ3/6 calculations. The use of DATA0.FM6 is a deviation from Brush et al., (2012) which specifies DATA0.FM1 (Xiong, 2011) as the thermodynamic database.

Notice that as Brush et al. (2012, Subsection 4.3) anticipated using Steps 2a and 2b for the current analysis, combination of these two steps into Step 2 for this analysis was a deviation from AP-153, Rev. 1. See Brush et al. (2012, Subsection 4.3) for a description of Steps 2a and 2b.

All files are archived at "/data/cvs/CVSLIB/WIPP_EXTERNAL/ap153_files/CRA-2026-IS". Table 2 provides the location of the specific files.

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Table 2. Locations of the Excel Spreadsheets, I/O Files, etc., Used in the EQ3/6 Calculations for this Analysis.

Description or Title of File(s)	Location of File(s)
Spreadsheet *AP-153_Scaling of Solids_CRA-2026-IS.xlsx*	In zip file CRA-2026-IS_AP153R1.zip, /data/cvs/CVSLIB/WIPP_EXTERNAL/ap153_files/ CRA-2026-IS
Spreadsheet: *Conc_density_calcs_CRA-2026-IS.xlsx*	In zip file CRA-2026-IS_AP153R1.zip, /data/cvs/CVSLIB/WIPP_EXTERNAL/ap153_files/ CRA-2026-IS
EQ3/6 DB DATA0.FM6	In zip file CRA-2026-IS_AP153R1.zip, /data/cvs/CVSLIB/WIPP_EXTERNAL/ap153_files/ CRA-2026-IS
Excel macro *GetEQData_v101f.xls*	In zip file CRA-2026-IS_AP153R1.zip, /data/cvs/CVSLIB/WIPP_EXTERNAL/ap153_files/ CRA-2026-IS
EQ3/6 I/O files and Excel spreadsheets with extracted data	In zip file CRA-2026-IS_AP153R1.zip, /data/cvs/CVSLIB/WIPP_EXTERNAL/ap153_files/ CRA-2026-IS

The output was extracted from the EQ6 *.6o files by running the Excel macro "GetEQData_v101f.xls." This macro extracts all of the EQ6 output into an Excel spreadsheet.

All of our EQ3/6 input and output (I/O) files, the Excel macro GetEQData_v101f.xls, and the Excel spreadsheets that contain the output extracted with GetEQData_v101f.xls are in zip file CRA-2026-IS_AP153R1.zip.

2.2 Inputs

The baseline solubility model inputs include the brine compositions, brine physical properties (density and total dissolved solids), the organics concentrations, the actinide solubility controlling phases, and the mass (moles) of the important solid phases in the repository (halite, anhydrite, brucite, hydromagnesite5424, iron, and lead reactants). The EQ3/6 code is comprised of two separate codes, EQ3NR used for Step 1, and EQ6 used for Step 2, each of which requires different inputs. Step 1, EQ3NR, uses the brine compositions (Table 3), the organics input (Table 4), and the actinide solubility controlling phases and calculates the speciated solution composition and saturation index for all pertinent phases. For Step 2, the EQ6 code uses an output file of EQ3NR called a "pickup" file, which contains the initial solution information, EQ6 uses this composition and numerically titrates the reactants (Table 5) specified in the EQ6 input file, into this solution

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until the system reaches equilibrium, or until all of the reactants are expended. The resulting equilibrium final composition provides the chemical properties of the solution and the actinide concentrations that are used in PA.

The unreacted ERDA-6 and GWB [Brush et al., (2012) after Popielak et al. (1983) and Krumhansl et al. (1991); and Snider (2003), respectively] brine compositions that were used as input for the EQ3NR code are listed in Table 3.

Table 3. Input brine compositions, TDS, and densities used for the Baseline Solubility simulations.

	ERDA-6	GWB	
Na^+	4.87	3.53	Molarity
K^+	9.70E-02	4.67E-01	Molarity
Mg^{2+}	1.90E-02	1.02	Molarity
Ca^{2+}	1.20E-02	1.40E-02	Molarity
Cl^-	4.80	5.86	Molarity
HCO_3^-	1.60E-02	1.60E-02	Molarity
SO_4^{2-}	1.70E-01	1.77E-01	Molarity
B_{total} as $B(OH)_4^-$	6.30E-02	1.58E-01	Molarity
Br^-	1.10E-02	2.66E-02	Molarity
H^+	7.00	7.00	pmH
TDS[A]	310044.4	365079.6	mg/L
Density[A]	1.19938	1.2346	g/cm^3

A – The TDS and density values in Table 3 are not used in the EQ3NR input files because they do not account for the organic ligands. The EQ3NR input values may be found in the *Conc_density_calcs_CRA-2026-IS.xlsx* spreadsheet.

The initial value of the total inorganic carbon (TIC), represented as HCO_3^-, of both brines were set at 16 mM for this step because: (1) Popielak et al, (1983) reported that the average TIC content of ERDA-6 was 16 mM, (2) the initial TIC of GWB was not determined, so (3) it was assumed that the initial TIC content of GWB was equal to that of ERDA-6. The initial value of the TIC did not affect the values of the TIC predicted during for the equilibrium system. The pmH for both brines was set to 7.0. When using molar input values they must be scaled by the solution density which is calculated in the spreadsheet, *Conc_density_calcs_CRA-2026-IS.xlsx* and includes the concentrations of organic ligands.

In addition to the brine composition data (Table 3) the scaled organics concentrations (Table 4) are also used as input for EQ3NR (Domski, 2025b). The concentrations of acetate (CH_3COO^-), citrate ($(CH_2COO)_2C(OH)(COO)^{3-}$), EDTA (ethylenediaminetetraacetate, or $CH_2COO)_2N(CH_2)_2N(CH_2COO)_2)^{4-}$), and oxalate ($(COO)_2^{2-}$) dissolved in volumes of GWB and ERDA-6 that are 1 ×, 2 ×, 3 ×, 4 ×, and 5 × DBR volume, 6,314 m^3 (Brunell, 2025), are from Domski (2025b). Table 4 provides the concentrations of these organic ligands used for this analysis. Acetate, citrate, EDTA, and oxalate are the organic ligands in TRU waste that could form complexes with actinide elements and increase their solubilities.

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Table 4. Dissolved Concentrations of Organic Ligands (M) in the Minimum Brine Volume Required for a DBR and for Volumes That Are 2 ×, 3 ×, 4 ×, and 5 × the Minimum Volume.

Organic Ligand	Minimum Required for a DBR	2 × Minimum	3 × Minimum	4 × Minimum	5 × Minimum
Acetate	8.29E-02	4.15E-02	2.76E-02	2.07E-02	1.66E-02
Citrate	8.88E-03	4.44E-03	2.96E-03	2.22E-03	1.78E-03
EDTA	2.13E-04	1.06E-04	7.09E-05	5.31E-05	4.25E-05
Oxalate	3.08E-02	1.54E-02	1.03E-02	7.71E-03	6.17E-03

The final EQ3NR inputs are the solubility controlling phases used to set the An(III), An(IV), and An(V) concentrations. For An(III) the amorphous americium hydroxide phase, $Am(OH)_3(am)$, is set as solubility controlling phase. A discussion of the rationale for using this phase is provided in Domski (2023a).

The An(IV) model uses the amorphous form of thorium oxide, $ThO_2(am)$, as the solubility controlling phase. This phase has been used as the An(IV) solubility controlling phase since the CCA, and it is consistent with the thorium model included in the database.

The solubility controlling phase for An(V) since the CCA has been $KNpO_2CO_3$. Brush and Garner (2005) made the argument that dissolved An(V) releases do not affect the long-term performance of the WIPP, so this phase will continued to be used for the CRA-2026 IS.

Inputs for EQ6 include the pickup file (*.3p) generated in Step 1 by EQ3NR, and the total moles of each reactant phase (Table 5) to be included in the model. The reactant quantities are scaled to 1 kg of solvent water, the initial mass of water on which EQ3/6 operates; subsequent dissolution/precipitation reactions can add or remove water from the system. In a computation, documented in the spreadsheet, *AP-153_Scaling of Solids_CRA-2026-IS.xlsx*, the quantities of carbon (Van Soest, 2025b), brine, halite, anhydrite, brucite, hydromagnesite, hibbingite, and hydrocerussite used as inputs were calculated. The quantities will be present in the repository after it is filled and sealed but scaled down by the same factor used to scale down the quantity of water contained in the 6,314 m^3 of brine to 1 kg of water. These values can be found in PAIR 2024 (Van Soest 2025b).

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Discussion on the scaling of the geologic reactants and CH_AREA variable.

Table 5. Reactants (moles) in the Minimum Brine Volume Required for a DBR and for Volumes That Are 2 ×, 3 ×, 4 ×, and 5 × the Minimum Volume.

Total Carbon from CPR: 1.15E+09 moles

Total MgO: Total Carbon from CPR (1.15E+09 moles) x MgO excess factor (1.2) = 1.38E+09 moles

Reactant (mols)	Brine/Volume Factor	1x	2x	3x	4x	5x
Halite	GWB	1.23E+04	6.14E+03	4.09E+03	3.07E+03	2.45E+03
Halite	ERDA-6	1.20E+04	6.00E+03	4.00E+03	3.00E+03	2.40E+03
Anhydrite	GWB	5.85E+02	2.93E+02	1.95E+02	1.46E+02	1.17E+02
Anhydrite	ERDA-6	5.72E+02	2.86E+02	1.91E+02	1.43E+02	1.14E+02
Brucite	GWB	1.25E+02	6.27E+01	4.18E+01	3.13E+01	2.51E+01
Brucite	ERDA-6	1.23E+02	6.13E+01	4.09E+01	3.06E+01	2.45E+01
Hydromagnesite	GWB	2.51E+01	1.25E+01	8.36E+00	6.27E+00	5.01E+00
Hydromagnesite	ERDA-6	2.45E+01	1.23E+01	8.17E+00	6.13E+00	4.90E+00
Hibbingite	GWB	6.54E+01	3.27E+01	2.18E+01	1.63E+01	1.31E+01
Hibbingite	ERDA-6	6.39E+01	3.20E+01	2.13E+01	1.60E+01	1.28E+01
Hydrocerussite	GWB	5.70E-01	2.85E-01	1.90E-01	1.42E-01	1.14E-01
Hydrocerussite	ERDA-6	5.57E-01	2.79E-01	1.86E-01	1.39E-01	1.11E-01

In Table 5 the "Total carbon from CPR" represents the total moles of carbon in the CPR from the PAIR (see Table 5-5 and Table 5-7 in the "*IS PAIR-2024 R0 Tables.xlsx*" spreadsheet (Van Soest, 2025b), it is the sum of the "waste", "packaging", and "total emplaced and operational" values in both the contact handled (CH) and remote handled (RH) columns). It should be calculated as:

$$Total\ Carbon\ (moles) = \frac{[Mass_{Cellulose} + (REFCON{:}\,PLASFRAC\ \times Mass_{Plastic}) + Mass_Rubber]}{REFCON{:}\,MW_CELL}$$

REFCON:PLASFRAC is the mass (kg) ratio of plastics to equivalent carbon and has a value of 1.7. MW_CELL is the molecular weight of cellulose ($C_6H_{10}O_5$) normalized to one mole of carbon (162.1406 g/mol / 6 mol C/mol cellulose / 1000 g/kg = 2.7023E-02 kg/mol_carbon). The total moles of MgO are calculated by multiplying the total moles of carbon from the CPR by the MgO excess factor, 1.2, i.e. MgO_{moles}= 1.2 x Σ C_{moles}. The MgO excess factor is a safety factor to account for possible variations in the mass of CPR. Each mole of carbon in the CPR can generate one mole of CO_2, which can react with the MgO hydration product brucite to form hydromagnesite. The stoichiometry is different for the two reactions, five moles of carbon are

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required to form one mole of hydromagnesite5424. The total moles of carbon are shown in Table 5 and documented in the spreadsheet titled *AP-153_Scaling of Solids_CRA-2026-IS.xlsx*. Note, the density and total dissolved solids (TDS) values of the unreacted brines in Table 3 were used to calculate the solids scaling factor[3], which was used to calculate the scaled mass of the reactants in Table 4, for each brine volume. These density and TDS values do not include the organic ligands, however, the effect of the organic ligands on the moles of the reactants as presented in Table 4 when the ligands were included was negligible, furthermore, the reactants are present in excess meaning that small changes in their amounts had no impact on the final equilibrium chemistry.

The conceptual model assumption is that GWB, or ERDA-6, contacts and reacts with the geologic (halite and anhydrite), engineered barrier (MgO), and waste form (actinide phases, organics, CPR, steel, and lead) simultaneously. This supports the conceptual model assumption of chemical homogeneity and solubility equilibrium and allows for the assumption of instantaneous reactions (Wilson et al., 1996).

The same model input changes that were made for the RPPCR from CRA-2019 DPA were carried forward to the CRA-2026 IS baseline solubility calculations. The changes are outlined below, see Domski (2023a) for detailed discussions of these changes.

1) Lead and iron reactants, used for CRA-2026 IS are hydrocerussite ($2PbCO_3.Pb(OH)_2(s)$) and hibbingite ($Fe_2Cl(OH)_3$), respectively.

2) For CRA-2026 IS calcite ($CaCO_3$) was suppressed and aragonite was allowed to precipitate should it become saturated reaction-path simulations.

3) The magnesium oxy-chloride phase, Phase 5 ($Mg_3Cl(OH)_5{\cdot}4H_2O$), was suppressed based on the analysis of Domski and Nemer (2023).

4) The masses (moles) of the reactants were scaled to DBR volume for CRA-2026 IS.

5) The aqueous species $FeEDTA^{2-}$ was suppressed;

6) $FeCitrate^{-}$ and $FeOHCitrate^{2-}$ aqueous species were allowed in the CRA-2026 IS baseline solubility calculations;

7) $Am(OH)_3(am)$ was be used as the solubility controlling phase in Step 1, and $Am(OH)_3(s)$ was suppressed in Step 2.

The baseline solubility model includes three man-made components: 1) The MgO engineered barrier; 2) steel (100 percent represented as iron) waste containers; and 3) lead radiation shielding. These three components are represented in the model as four solid reacting phases: 1) The MgO engineered barrier system is represented as 50-50 by moles of Mg combination of brucite and

[3] Solid Scaling Factor $= 1/([\rho_{brine} - TDS] \times Vol_{DBR})$, ρ_{brine} = brine density (kg/m^3), TDS = brine total dissolved solids (kg/m^3), Vol_{DBR} = DBR volume (m^3)

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hydromagnesite; 2) the iron comprising the waste containers is represented as hibbingite; and 3) and the lead shielding is represented as hydrocerussite. Each of these four solid phases requires water (brine) to form. However, inflows and outflows of brine are not calculated in EQ3/6. Rather they are calculated in PA, within the BRAGFLO code. A one-way loose coupling between the two models is achieved by producing a table of solubilities in EQ3/6 from a minimum brine volume required for a release, or one DBR, increasing to a maximum of five DBR volumes with solubilities calculated at 1x, 2x, 3x, 4x, and 5x the minimum volume. That table is then used as a lookup table in PA to determine the solubilities based on the amount of brine in the repository at the time of a release.

The sources of this water for hydration of the model components in the repository may originate from water vapor in the closed repository, brine draining from the disturbed rock zone (DRZ), brine flow from the Salado Formation, and brine entering the repository from a Castile Formation and/or the Culebra member of the Rustler Formation via a borehole penetrating these formations. This is discussed further in Section PA-4.2 of Appendix PA (DOE, 2019).

The masses of the geologic reactants, halite and anhydrite, used in Step 2 are calculated based on the volume of the disturbed-rock zone (DRZ) calculated from the area of the repository footprint and the DRZ dimensions. From King (2021) "…vertical extent of the DRZ is assumed to remain the same, 11.95 m above the repository and 2.23 m below the repository." The repository area (PA property CH_AREA) for the current analysis was provided in Table 1 of Brunell (2025) which also provides these values for the RPPCR, CRA-2026 FS, and CRA-2026 IS. For the CRA-2026 FS baseline solubility model (Domski, 2025a) the RPPCR CH_AREA was used, as documented in King (2021), to calculate the amounts of halite and anhydrite. The RPPCR CH_AREA was used because Brunell (2025) was not available at the time that the CRA-2026 FS analysis was performed. This had no effect on the baseline solubility results as is discussed in Section 3.

3 RESULTS

The output from Step 2 consisted of EQ6 output files (*.6o) for each brine and brine volume, which detail the chemistry of each reaction step, and includes the calculated moles of solids that dissolved and/or precipitated, speciated solution composition, the total dissolved elements; and the intensive solution properties as the reaction progressed. The Excel macro "GetEQData_v101f.xls." was used to extract the actinide elemental concentrations and species concentrations which are presented below.

Table 6 provides the compositions; the solubilities of Th(IV), Np(V), and Am(III); and parameters such as f_{CO_2}, pcH, and TIC for volumes of GWB that are 1 ×, 2 ×, 3 ×, 4 ×, and 5 × 6,314 m^3, the minimum brine volume required for a direct brine release (DBR) from the repository (Brunell, 2025). Table 7 provides comparable information for ERDA-6. Brush et al. (2012, Subsection 2.1.2) described the solid phases that will control the compositions and other conditions in these brines, and the solubilities of the important actinides in TRU waste, after these brines and solids equilibrate. In particular, the brucite-hydromagnesite carbonation reaction will control f_{CO_2} and the total inorganic carbon content of the brines.

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Table 8 shows the dissolved species distributions predicted for Th(IV) in the minimum volume and 5 × the minimum volume of GWB. Table 9 shows the species distributions for Th(IV) in the minimum volume and 5 × the minimum volume of ERDA-6 . Tables 10, 11, 12, and 13 provide comparable information for Np(V) and Am(III).

Tables 14 and 15 show the solid phase budgets for the minimum brine volume case (1x) for GWB and ERDA-6, respectively. The tables provide the initial and final masses (moles) on an EQ3/6 scale, for both the reactant and product phases, as well as their change in mass (moles) for each phase. Negative values of "Delta Mass" indicates dissolution, and positive values indicate precipitation.

The CRA-2026 IS has the same product phases as the CRA-2026 FS (Domski, 2025a) for both brines, while compared to the results of the CRA-2019 DPA (Domski and Sisk-Scott, 2019) the RPPCR (Domski, 2023a) and the CRA-2026 IS had fewer product phase minerals for each brine type. For GWB the products included Phase 3, whewellite, and the An(V) solubility controlling phase $KNpO_2CO_3$ (Table 14), and for ERDA-6 which included whewellite, and the An(V) solubility controlling phase $KNpO_2CO_3$ (Table 15).

Note from Tables 14 and 15 that the stable An(III) phase is $AmOHCO_3(s)$ for both brine types, this was predicted by Domski (2022) when the amorphous americium hydroxide phase is used to set the An(III) concentration in Step 1 of the simulation, and the less soluble form [$Am(OH)_3(s)$] is suppressed. This point was discussed at the DOE technical exchange with the EPA at the October 25, 2022 meeting.

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Table 6. EQ3/6 Predictions of the Compositions and Solubilities of Th(IV), Np(V), and Am(III) in Five Different Volumes of GWB (M Unless Otherwise Noted).

Element or Property	1 × Minimum[A]	2 × Minimum	3 × Minimum	4 × Minimum	5 × Minimum
B(III)(aq)	0.188	0.186	0.186	0.186	0.185
Na(I)(aq)	4.31	4.36	4.38	4.39	4.40
Mg(II)(aq)	0.932	0.845	0.816	0.802	0.794
K(I)(aq)	0.554	0.550	0.549	0.548	0.548
Ca(II)(aq)	0.013	0.013	0.013	0.013	0.013
Fe(II)(aq)	1.50E-04	8.93E-05	6.94E-05	5.95E-05	5.35E-05
S(VI)(aq)	0.241	0.222	0.215	0.212	0.210
Cl(-I)(aq)	4.75	4.89	4.94	4.96	4.97
Br(-I)(aq)	03.16E-02	3.13E-02	3.13E-02	3.12E-02	3.12E-02
Pb(II)(aq)	1.12E-02	1.13E-02	1.13E-02	1.14E-02	1.14E-02
Th(IV)(aq)	5.34E-08	5.34E-08	5.33E-08	5.34E-08	5.34E-08
Np(V)(aq)	9.75E-07	6.88E-07	5.81E-07	5.24E-07	4.90E-07
Am(III)(aq)	1.45E-05	7.88E-06	5.45E-06	4.20E-06	3.43E-06
f_{CO_2} (atm)	2.02E-06	2.02E-06	2.02E-06	2.02E-06	2.02E-06
Ionic Strength (m)	8.08	7.98	7.95	7.93	7.92
pH[B]	8.76	8.75	8.74	8.74	8.74
pcH	9.34	9.35	9.36	9.36	9.36
RH (%)[C]	73.00%	73.09%	73.12%	73.13%	73.14%
TIC[D]	2.34E-04	2.33E-04	2.33E-04	2.32E-04	2.32E-04

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Mass of Water (kg)	0.734	0.740	0.742	0.743	0.743
m:M[E]	1.148	1.147	1.147	1.147	1.147

Footnotes for Table 6:

A. Based on a minimum brine volume of 6,314 m^3 (Brunell, 2025)
B. The Pitzer scale is an unofficial pH scale consistent with pH values calculated using single-ion activity coefficients based on the Pitzer activity-coefficient model for brines and evaporite minerals of Harvie et al. (1984), extended to include Nd(III), Am(III), and Cm(III); Th(IV); and Np(V). T. J. Wolery of Lawrence Livermore National Laboratory (LLNL) in Livermore, CA, proposed the term "Pitzer scale" unofficially.
C. RH = relative humidity. The value of the RH divided by 100 yields the value of the activity of H_2O in GWB.
D. TIC = total inorganic C.
E. m:M = molality:Molarity ratio

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Table 7. EQ3/6 Predictions of the Compositions of and Solubilities of Th(IV), Np(V), and Am(III) in Five Different Volumes of ERDA-6 (M Unless Otherwise Noted).

Element or Property	1 × Minimum[A]	2 × Minimum	3 × Minimum	4 × Minimum	5 × Minimum
B(III)(aq)	0.062	0.062	0.062	0.062	0.062
Na(I)(aq)	4.93	5.03	5.07	5.09	5.10
Mg(II)(aq)	0.546	0.446	0.413	0.397	0.387
K(I)(aq)	0.096	0.096	0.096	0.096	0.096
Ca(II)(aq)	0.013	0.013	0.013	0.013	0.013
Fe(II)(aq)	1.72E-04	1.03E-04	7.78E-05	6.47E-05	5.66E-05
S(VI)(aq)	1.98E-01	1.83E-01	1.78E-01	1.76E-01	1.74E-01
Cl(-I)(aq)	4.86	4.97	5.00	5.02	5.03
Br(-I)(aq)	1.09E-02	1.09E-02	1.09E-02	1.09E-02	1.09E-02
Pb(II)(aq)	6.51E-03	5.83E-03	5.58E-03	5.45E-03	5.38E-03
Th(IV)(aq)	5.63E-08	5.69E-08	5.71E-08	5.72E-08	5.73E-08
Np(V)(aq)	4.01E-06	2.64E-06	2.17E-06	1.93E-06	1.79E-06
Am(III)(aq)	1.44E-05	8.02E-06	5.59E-06	4.32E-06	3.54E-06
fCO_2 (atm)	2.02E-06	2.02E-06	2.02E-06	2.02E-06	2.02E-06
Ionic Strength (m)	7.24	7.13	7.09	7.08	7.07
pH[B]	8.80	8.81	8.82	8.82	8.82
pcH	9.41	9.44	9.45	9.46	9.46
RH (%)[C]	74.23%	74.37%	74.42%	74.44%	74.46%
TIC[D]	2.42E-04	2.44E-04	2.46E-04	2.47E-04	2.47E-04

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Mass of Water (kg)	0.892	0.892	0.893	0.893	0.893
m:M[E]	1.136	1.136	1.136	1.135	1.135

Footnotes for Table 7:

A. Based on a minimum brine volume of 6,314 m^3 (Brunell, 2025)
B. The Pitzer scale is an unofficial pH scale consistent with pH values calculated using single-ion activity coefficients based on the Pitzer activity-coefficient model for brines and evaporite minerals of Harvie et al. (1984), extended to include Nd(III), Am(III), and Cm(III); Th(IV); and Np(V). T. J. Wolery of Lawrence Livermore National Laboratory (LLNL) in Livermore, CA, proposed the term "Pitzer scale" unofficially.
C. RH = relative humidity. The value of the RH divided by 100 yields the value of the activity of H_2O in ERDA-6.
D. TIC = total inorganic C.
E. molality:Molarity ratio

Tables 8 – 13 provide the +IV, +V, and +III actinide aqueous speciation data for GWB and ERDA-6 for the minimum brine volume (1x) case and the maximum brine volume (5x) cases. The tables provide the molarity of each species and the percent of the total actinide concentration of each species. Tables 8 and 9 provide the GWB and ERDA-6 Th(IV) speciation information, respectively. Tables 10 and 11 provide the GWB and ERDA-6 Np(V) speciation information, respectively. Tables 12 and 13 provide the GWB and ERDA-6 Am(III) speciation information, respectively. Note the species for each brine volume in Tables 8 – 13 are sorted in descending order by concentration and the species concentrations are typically not the same between the 1x and 5x volumes, thus, the species names are provided for both volumes. This method of reporting was chosen to elucidate that the speciation changes as the volume of brine changes.

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Table 8. Comparisons of Distributions of Dissolved Th(IV) Species in the Minimum Volume and 5 × the Minimum Volume of GWB. Percentages of solubilities < 0.01 were not reported. The solubility-controlling solid was hydrous, amorphous ThO_2.

GWB, minimum volume			GWB, 5 × minimum volume		
Th(IV) Species	Concentration (M)	Percent of Solubility	Th(IV) Species	Concentration (M)	Percent of Solubility
$Th(OH)_4(aq)$	4.50E-08	84.26%	$Th(OH)_4(aq)$	4.52E-08	84.72%
$Th(OH)_3(CO_3)^-$	8.40E-09	15.74%	$Th(OH)_3(CO_3)^-$	8.15E-09	15.28%
ThEDTA(aq)	1.81E-16		ThEDTA(aq)	3.82E-17	
$Th(CO_3)_5^{6-}$	5.36E-17		$Th(CO_3)_5^{6-}$	1.85E-17	
$Th(SO_4)_3^{2-}$	2.11E-17		$Th(SO4)_3^{2-}$	1.29E-17	
$Th(Acetate)_2^{2+}$	1.28E-18		$Th(SO_4)_2(aq)$	3.24E-19	
$ThCitrate^+$	7.72E-19		$ThCitrate^+$	1.41E-19	
$Th(SO_4)_2(aq)$	5.03E-19		$Th(Acetate)_2^{2+}$	3.94E-20	
$ThAcetate^{3+}$	7.37E-20		$ThAcetate^{3+}$	7.76E-21	
$ThOxalate^{2+}$	4.50E-22		$ThOxalate^{2+}$	2.67E-22	
Th^{4+}	1.76E-23		Th^{4+}	7.62E-24	
Total:	5.34E-08	100.00%	Total:	5.34E-08	100.00%

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Table 9. Comparisons of Distributions of Dissolved Th(IV) Species in the Minimum Volume and 5 × the Minimum Volume of ERDA-6. Percentages of solubilities < 0.01 were not reported. The solubility-controlling solid was hydrous, amorphous ThO_2.

ERDA-6, minimum volume			ERDA-6, 5 × minimum volume		
Th(IV) Species	Concentration (M)	Percent of Solubility	Th(IV) Species	Concentration (M)	Percent of Solubility
$Th(OH)_4(aq)$	4.70E-08	83.39%	$Th(OH)_4(aq)$	4.73E-08	82.61%
$Th(OH)_3CO_3^-$	9.36E-09	16.61%	$Th(OH)_3CO_3^-$	9.96E-09	17.39%
ThEDTA(aq)	1.59E-16	0.00%	ThEDTA(aq)	3.10E-17	
$Th(SO_4)_3^{2-}$	9.83E-18	0.00%	$Th(SO_4)_3^{2-}$	4.00E-18	
$Th(CO_3)_5^{6-}$	7.16E-18	0.00%	$Th(CO_3)_5^{6-}$	1.81E-18	
$ThCit^+$	1.13E-18	0.00%	$ThCit^+$	1.81E-19	
$ThAc_2^{2+}$	6.48E-19	0.00%	$Th(SO_4)_2(aq)$	7.26E-20	
$Th(SO_4)_2(aq)$	1.56E-19	0.00%	$ThAc_2^{2+}$	1.90E-20	
$ThAc^{3+}$	2.48E-20	0.00%	$ThAc^{3+}$	2.43E-21	
$ThOx^{2+}$	3.17E-22	0.00%	$ThOx^{2+}$	1.47E-22	
Th^{4+}	6.46E-24	0.00%	Th^{4+}	2.29E-24	
Total:	5.64E-08[A]	100.00%	Total:	5.73E-08	100.00%

A - The Th(IV) total concentration in Table 9 differs from that in Table 7 (5.63E-08 M) due to an EQ6 internal rounding discrepancy in the Th-species concentrations. For compliance purposes the value in Table 7 will used in PA.

Tables 8 and 9 show that the most important aqueous species for Th(IV) is $Th(OH)_4(aq)$ at ~83 - 84%, and $Th(OH)_3CO_3^-$ ~14 - 16%. The aqueous species formed with organic ligands are inconsequential with regard to the Th(IV) solubility. The change in the total Th(IV) concentration is negligible for the two brines

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Table 10. Comparisons of Distributions of Dissolved Np(V) Species in the Minimum Volume and 5 × the Minimum Volume of GWB. Percentages of solubilities < 0.01 were not reported. The solubility-controlling solid was $KNpO_2CO_3$.

GWB, minimum volume			GWB, 5 × minimum volume		
Np(V) Species	Concentration (M)	Percent of Solubility	Np(V) Species	Concentration (M)	Percent of Solubility
$NpO_2Ac(aq)$	6.24E-07	63.94%	NpO_2^+	1.96E-07	39.93%
NpO_2^+	1.98E-07	20.34%	$NpO_2Ac(aq)$	1.43E-07	29.17%
$NpO_2CO_3^-$	7.29E-08	7.48%	$NpO_2CO_3^-$	8.03E-08	16.40%
$NpO_2Oxalate^-$	7.29E-08	7.47%	$NpO_2Oxalate^-$	6.51E-08	13.29%
$NpO_2OH(aq)$	4.43E-09	0.45%	$NpO_2OH(aq)$	5.02E-09	1.03%
$NpO_2Citrate^{2-}$	2.73E-09	0.28%	$NpO_2Citrate^{2-}$	5.44E-10	0.11%
$NpO_2(CO_3)_2^{3-}$	2.93E-10	0.03%	$NpO_2(CO_3)_2^{3-}$	3.51E-10	0.07%
NpO_2EDTA^{3-}	1.58E-11		$NpO_2(OH)_2^-$	7.92E-12	
$NpO_2(OH)_2^-$	7.05E-12		NpO_2EDTA^{3-}	2.87E-12	
$NpO_2(CO_3)_3^{5-}$	3.87E-14		$NpO_2(CO_3)_3^{5-}$	8.42E-14	
NpO_2HEDTA^{2-}	2.90E-14		NpO_2HEDTA^{2-}	6.07E-15	
$NpO_2H_2EDTA^-$	3.95E-18		$NpO_2H_2EDTA^-$	8.85E-19	
Total:	9.75E-07	100.00%	Total:	4.90E-07	100.00%

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Table 11. Comparisons of Distributions of Dissolved Np(V) Species in the Minimum Volume and 5 × the Minimum Volume of ERDA-6. Percentages of solubilities < 0.01 were not reported. Percentages do not add up to 100% because concentrations were rounded to three significant figures before calculating percentages. The solubility-controlling solid was $KNpO_2CO_3$.

ERDA-6, minimum volume			ERDA-6, 5 × minimum volume		
Np(V) Species	Concentration (M)	Percent of Solubility	Np(V) Species	Concentration (M)	Percent of Solubility
$NpO_2Ac(aq)$	2.53E-06	63.07%	NpO_2^+	6.21E-07	34.81%
NpO_2^+	7.71E-07	19.24%	$NpO_2Ac(aq)$	5.20E-07	29.12%
$NpO_2CO_3^-$	4.01E-07	10.02%	$NpO_2CO_3^-$	4.14E-07	23.17%
$NpO_2Oxalate^-$	2.68E-07	6.69%	NpO_2Ox^-	2.03E-07	11.37%
$NpO_2(OH)(aq)$	2.21E-08	0.55%	$NpO_2(OH)(aq)$	2.18E-08	1.22%
NpO_2Cit^{2-}	1.49E-08	0.37%	NpO_2Cit^{2-}	2.85E-09	0.16%
$NpO_2(CO_3)_2^{3-}$	2.23E-09	0.06%	$NpO_2(CO_3)_2^{3-}$	2.67E-09	0.15%
NpO_2EDTA^{3-}	4.20E-11		$NpO_2(OH)_2^-$	4.10E-11	
$NpO_2(OH)_2^-$	3.84E-11		NpO_2EDTA^{3-}	6.25E-12	
$NpO_2(CO_3)_3^{5-}$	1.00E-12		$NpO_2(CO_3)_3^{5-}$	1.76E-12	
NpO_2HEDTA^{2-}	1.43E-13		NpO_2HEDTA^{2-}	2.73E-14	
$NpO_2H_2EDTA^-$	3.17E-17		$NpO_2H_2EDTA^-$	6.34E-18	
Total:	4.01E-06	100.00%		1.79E-06	100.00%

The Np(V) speciation for the minimum volume (1x) case for GWB and ERDA-6 (Tables 10 and 11) is distributed over seven species with ~98% of the Np(V) distributed, between four species, $NpO_2Ac(aq)$, NpO_2^+, $NpO_2CO_3^-$, and $NpO_2Oxalate^-$ in descending order. For the maximum volume case (5x) the total Np(V) concentration is distributed over the same species as the 1x case but in a different order for each brine and with a more equal distribution among the species.

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Table 12. Comparisons of Distributions of Dissolved Am(III) Species in the Minimum Volume and 5 × the Minimum Volume of GWB. Percentages of solubilities < 0.01 were not reported. Percentages do not add up to 100% because concentrations were rounded to three significant figures before calculating percentages. The solubility-controlling solid was $AmOHCO_3(c)$.

GWB, minimum volume			GWB, 5 × minimum volume		
Am(III) Species	Concentration (M)	Percent of Solubility	Am(III) Species	Concentration (M)	Percent of Solubility
$AmEDTA^-$	1.43E-05	98.52%	$AmEDTA^-$	3.17E-06	92.54%
$Am(OH)_2^+$	1.69E-07	1.16%	$Am(OH)_2^+$	2.36E-07	6.89%
$AmAc^{2+}$	2.68E-08	0.18%	$Am(OH)^{2+}$	8.52E-09	0.25%
$AmOH^{2+}$	8.55E-09	0.06%	$AmAc^{2+}$	5.76E-09	0.17%
AmCit(aq)	8.01E-09	0.06%	AmCit(aq)	2.01E-09	0.06%
$Am(OH)_3(aq)$	1.49E-09	0.01%	$Am(OH)_3(aq)$	1.71E-09	0.05%
$AmCO_3^+$	8.28E-10	0.01%	$AmCO_3^+$	8.22E-10	0.02%
$AmSO_4^+$	4.07E-10		$AmSO_4^+$	3.58E-10	0.01%
$Am(CO_3)_2^-$	2.20E-10		$Am(CO_3)_2^-$	2.17E-10	0.01%
Am^{3+}	1.11E-10		Am^{3+}	1.06E-10	
$Am(SO_4)_2^-$	8.34E-11		$AmOx^+$	6.26E-11	
$AmOx^+$	6.65E-11		$Am(SO_4)_2^-$	6.15E-11	
$Am(CO_3)_3^{3-}$	3.82E-11		$Am(CO_3)_3^{3-}$	3.45E-11	
$AmCl^{2+}$	1.75E-11		$AmCl^{2+}$	1.26E-11	
$Am(CO_3)_4^{5-}$	1.20E-12		$Am(CO_3)_4^{5-}$	1.11E-12	

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Table 12. Comparisons of Distributions of Dissolved Am(III) Species in the Minimum Volume and 5 × the Minimum Volume of GWB (continued). Percentages of solubilities < 0.01 were not reported. Percentages do not add up to 100% because concentrations were rounded to three significant figures before calculating percentages. The solubility-controlling solid was $AmOHCO_3$(c) (continued).

GWB, minimum volume			GWB, 5 × minimum volume		
Am(III) Species	Concentration (M)	Percent of Solubility	Am(III) Species	Concentration (M)	Percent of Solubility
$AmCl_2^+$	9.57E-13		$AmCl_2^+$	6.69E-13	
Total:	1.45E-05	100.00%	Total:	3.43E-06	100.00%

Table 13. Comparisons of Distributions of Dissolved Am(III) Species in the Minimum Volume and 5 × the Minimum Volume of ERDA-6. Percentages of solubilities < 0.01 were not reported. Percentages may not add up to 100% because concentrations were rounded to three significant figures before calculating percentages. The solubility-controlling solid was $AmOHCO_3$(c).

ERDA-6, minimum volume			ERDA-6, 5 × minimum volume		
Am(III) Species	Concentration (M)	Percent of Solubility	Am(III) Species	Concentration (M)	Percent of Solubility
$AmEDTA^-$	1.41E-05	98.20%	$AmEDTA^-$	3.24E-06	91.70%
$Am(OH)_2^+$	2.30E-07	1.59%	$Am(OH)_2^+$	2.81E-07	7.95%
$AmAc^{2+}$	1.21E-08	0.08%	$AmOH^{2+}$	5.16E-09	0.15%
AmCit(aq)	7.83E-09	0.05%	$AmAc^{2+}$	2.18E-09	0.06%
$AmOH^{2+}$	6.20E-09	0.04%	$Am(OH)_3$(aq)	1.94E-09	0.05%
$Am(OH)_3$(aq)	1.67E-09	0.01%	AmCit(aq)	1.71E-09	0.05%
$AmCO_3^+$	7.36E-10	0.01%	$AmCO_3^+$	6.65E-10	0.02%

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ERDA-6, minimum volume			ERDA-6, 5 × minimum volume		
Am(III) Species	Concentration (M)	Percent of Solubility	Am(III) Species	Concentration (M)	Percent of Solubility
$Am(CO_3)_2^-$	2.57E-10		$Am(CO_3)_2^-$	2.85E-10	0.01%
$AmSO_4^+$	2.23E-10		$AmSO_4^+$	1.50E-10	
Am^{3+}	7.01E-11		Am^{3+}	5.19E-11	
$AmOx^+$	5.41E-11		$AmOx^+$	3.85E-11	
$Am(SO_4)_2^-$	3.29E-11		$Am(CO_3)_3^{3-}$	3.19E-11	
$Am(CO_3)_3^{3-}$	3.11E-11		$Am(SO_4)_2^-$	1.91E-11	
$AmCl^{2+}$	6.78E-12		$AmCl^{2+}$	3.86E-12	
$AmCl_2^+$	3.05E-13		$Am(CO_3)_4^{5-}$	1.78E-13	
$Am(CO_3)_4^{5-}$	2.69E-13		$AmCl_2^+$	1.64E-13	
	1.44E-05	100.00%		3.54E-06	100.00%

The Am(III) speciation for GWB and ERDA-6 are shown in Tables 12 and 13. The most important Am(III) species is $AmEDTA^-$ followed by second hydrolysis species $Am(OH)_2^+$ for both the minimum and maximum volume cases. The 5x minimum volume case shows that as the EDTA budget decreases the Am(III) concentration decreases by nearly factor of 10.

The solids budget, total reactant and product masses, for the GWB and ERDA-6 brines are provided in Table 14 for GWB, and Table 15 for ERDA-6.

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Table 14. Solid budgets for the reactant and product phases at the initiation of Step 2 and for the final equilibrium for GWB brine with the repository solids. Note: Positive values of delta mass indicate precipitation, and negative indicate dissolution.

Phase	Reactant/ Product	Initial Mass (moles)	Final Mass (moles)	Delta Mass (moles)
Halite	Reactant	12300.00	12300.00	0.00
Anhydrite	Reactant	585.00	584.97	-0.03
Brucite	Reactant	125.00	121.92	-3.08
Hydromagnesite5424	Reactant	25.10	24.98	-0.12
Hibbingite	Reactant	65.40	65.40	0.00
Hydrocerussite	Reactant	0.5700	0.5668	-3.16E-03
$AmOHCO_3(c)$	Product	1.60E-02	4.91E-01	4.75E-01
$ThO_2(am)$	Product	2.89E-08	3.84E-08	9.47E-09
$KNpO_2CO_3$	Product	0.00E+00	1.19E-05	1.19E-05
Phase 3	Product	0.00	1.95	1.95
Whewellite	Product	0.00	2.96E-02	2.96E-02

Table 15. Solid budgets for the reactant and product phases at the initiation of Step 2 and for the final equilibrium for ERDA-6 brine with the repository solids. Note: Positive values of delta mass indicate precipitation, and negative indicate dissolution.

Phase	Reactant/ Product	Initial Mass (moles)	Final Mass (moles)	Delta Mass (moles)
Halite	Reactant	12000.00	12000.00	0.00
Anhydrite	Reactant	572.00	571.97	-0.03
Brucite	Reactant	123.00	122.89	-0.11
Hydromagnesite5424	Reactant	24.50	24.41	-0.09
Hibbingite	Reactant	63.90	63.90	0.00

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Phase	Reactant/ Product	Initial Mass (moles)	Final Mass (moles)	Delta Mass (moles)
Hydrocerussite	Reactant	0.56	0.55	-2.20E-03
$AmOHCO_3(c)$	Product	1.60E-02	3.62E-01	3.46E-01
$ThO_2(am)$	Product	0.00	6.66E-08	6.66E-08
$KNpO_2CO_3$	Product	0.00	2.29E-05	2.29E-05
Whewellite	Product	0.00	3.00E-02	3.00E-02

The most abundant reactants are the geologic components halite and anhydrite (see Tables 5, 14, and 15). The results show that for both the GWB and ERDA-6 brines halite neither dissolves nor precipitates and only a small amount, less than 0.05 mole of anhydrite dissolves. This indicates that halite and anhydrite were at, or were very close to equilibrium with the solutions throughout the reaction path, and that the simulations are not sensitive to the initial masses of these reactants.

The solids inventories for GWB and ERDA-6 show that the stable An(III) phase was $AmOHCO_3(c)$, and not $Am(OH)_3(am)$ which was used in Step 1 to set the An(III) concentration. Domski (2022) showed that at the expected WIPP conditions, water activity and $fCO_2(g)$, the americium hydroxy-carbonate phase, $AmOHCO_3(c)$, would be stable and not the amorphous hydroxide phase. Additionally, Phase 3 was stable in the GWB equilibrium mineral assemblage and absent from the ERDA-6 assemblage. The higher initial magnesium concentration (Table 3) leads to the formation of Phase 3 in GWB.

Table 16 and 17 compares the CRA-2026 IS solubilities of Th(IV), Np(V), and Am(III) in GWB and ERDA-6, predicted for the 1x brine volume case with those for the CRA-2014 PA, CRA-2019 DPA, RPPCR, and CRA-2026 FS. Table 14 and 15 also compares the values of f_{CO_2} and pH predicted for these compliance-related calculations.

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Table 16. Comparison of GWB Actinide Solubilities (M), f_{CO_2} (atm), and pH (Pitzer scale) from the CRA-2014 PA, CRA-2019 DPA, RPPCR, CRA-2026 FS, and CRA-2026 IS.

Property or Actinide Oxidation State	CRA-2014 PA ($GWB_{min.\ vol.}$, Hydromagnesite, with Organics, All Vectors)[A]	CRA-2019 DPA ($GWB_{min.\ vol.}$,, Hydromagnesite, with Organics, Pb, Fe All Vectors)[B]	RPPCR ($GWB_{min.\ vol.}$,, Hydromagnesite, with Organics, Pb, Fe All Vectors)[C]	CRA-2026 FS ($GWB_{min.\ vol.}$,, Hydromagnesite, with Organics, Pb, Fe All Vectors)[D]	CRA-2026 IS ($GWB_{min.\ vol.}$,, Hydromagnesite, with Organics, Pb, Fe All Vectors)[E]
—					
Th(IV)	6.05E-08	5.45E-08	5.34E-08	5.34E-08	5.34E-08
Np(V)	2.77E-07	4.02E-07	4.95E-07	7.97E-07	9.75E-07
Am(III)	2.59E-06	1.63 E-07	3.40E-06	1.14E-05	1.45E-05
f_{CO_2}	3.14E-06	2.02E-06	2.02E-06	2.02E-06	2.02E-06
pH	8.82	8.82	8.74	8.75	8.76

A. Brush and Domski (2013)
B. Domski and Sisk-Scott (2019)
C. Domski (2023a)
D. Domski (2025a)
E. Current Study

Table 17. Comparison of ERDA-6 Actinide Solubilities (M), f_{CO_2} (atm), and pH (Pitzer scale) from the CRA-2014 PA, CRA-2019 DPA, RPPCR, CRA-2026 FS, and CRA-2026 IS.

Property or Actinide Oxidation State	CRA-2014 PA (ERDA-$6_{min.\ vol.}$, Hydromagnesite, with Organics, All Vectors)[A]	CRA-2019 DPA (ERDA-$6_{min.\ vol.}$, Hydromagnesite, Pb, Fe with Organics, All Vectors)[B]	RPPCR (ERDA-$6_{min.\ vol.}$,, Hydromagnesite, with Organics, Pb, Fe All Vectors)[C]	CRA-2026 FS (ERDA-$6_{min.\ vol.}$,, Hydromagnesite, with Organics, Pb, Fe All Vectors)[D]	CRA-2026 IS (ERDA-$6_{min.\ vol.}$,, Hydromagnesite, with Organics, Pb, Fe All Vectors)[E]
Th(IV)	7.02E-08	5.44E-08	5.73E-08	5.67E-08	5.63E-08
Np(V)	8.76E-07	1.20E-06	1.80E-06	3.14E-06	4.01E-06
Am(III)	1.48E-06	1.78E-07	3.51E-06	1.15E-05	1.44E-05
f_{CO_2}	3.14E-06	2.02E-06	2.02E-06	2.02E-06	2.02E-06
pH	8.99	8.82	8.82	8.80	8.80

A. Brush and Domski (2013)
B. Domski and Sisk-Scott (2019)
C. Domski (2023a)
D. Domski (2025a)
E. Current Study.

4 CONCLUSIONS

This analysis report provides the new baseline solubilities of An(III), An(IV), and An(V), in two standard Waste Isolation Pilot Plant (WIPP) brines as a function of the volumes of these brines in the interim-state repository. The two standard brines used in this analysis are Generic Weep Brine (GWB) and ERDA-6. GWB represents intergranular Salado Formation (Fm.) brines at or near the stratigraphic horizon of the repository. ERDA-6 is representative of fluids in brine reservoirs in the Castile Fm.

The CRA-2026 IS baseline solubility model differs from the RPPCR and CRA-2026 FS baseline solubility model (Domski, 2023a and 2025a) in two ways: 1) The CRA-2026 IS was based on a new DBR volume (Brunell, 2025) which affects the scaling of the reactants, both the organic ligands and the solid phase reactants, used in the solubility model; and 2) a new inventory was issued for CRA-2026 IS (Van Soest, 2025b) which provides updated inventories for the organic ligands and reactants used in the solubility model.

Tables 6 and 7 (see Section 3 above) provide the equilibrium aqueous compositions; the actinide solubilities, and the intensive solution properties for GWB and ERDA-6 at the five brine volumes, respectively.

Tables 8 and 9 (Section 3) shows the dissolved species distributions predicted for Th(IV) in the minimum volume and 5 × the minimum volume of GWB and ERDA-6, respectively. Tables 10, 11, 12 and 13 provide comparable information for Np(V) and Am(III).

Tables 16 and 17 (Section 3) compare the solubilities of Th(IV), Np(V), and Am(III) predicted for the minimum brine volume of 6,314 m^3 from this study compared with those predicted for the CRA-2014 PA, CRA-2019 DPA, RPPCR, and the CRA-2026 FS. Tables 16 and 17 also compare the values of f_{CO_2} and pH predicted for these compliance-related calculations.

The dissolved An(IV) concentrations for the two brines for the CRA-2026 IS (≈ 5.3 – 5.6E-08 M) are similar to the those for the CRA-2026 FS, RPPCR, the CRA-2019 DPA and the CRA-2014 PA (≈ 5.3 – 7.0E-08 M) (Tables 16 and 17). The primary aqueous species for An(IV) for WIPP conditions is not an organic species, but rather a hydroxide and hydroxy-carbonate species which are unaffected by the effects of the smaller DBR volume, i.e., the organic ligand concentrations.

The total An(V) concentration showed a modest increase for the CRA-2026 IS compared to the CRA-2026 FS, RPPCR, the CRA-2019 DPA and the CRA-2014 PA (Tables 16 and 17). The cause of this increase was the increased concentrations of acetate and oxalate due to the smaller DBR volume which comprised a significant fraction of the An(V) aqueous species.

The An(III) concentrations calculated for the CRA-2026 IS increased compared to the CRA-2026 FS, RPPCR, the CRA-2019 DPA and the CRA-2014 PA (Tables 16 and 17). The decrease in the DBR volume by a factor of approximately 5.4 compared to the RPPCR is the cause of the increase in the organic ligand concentrations. Table 18 shows the total moles and concentrations of the organic ligands for the RPPCR, CRA-2026 FS, and the CRA-2026 IS and reveals that the total moles (mass) of the ligands was nearly the same for all three PAs. However, Table 18 also shows

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that their concentrations increased significantly as the DBR volume decreased. This translated directly to the increased An(III) concentration as $AmEDTA^-$ is the primary Am(III) aqueous species for Am(III).

Table 18. Comparison of the organic ligand total moles and concentrations for the RPPCR (Table 5, Domski, 2023b), CRA-2026 FS (Table 5, Domski, 2025d), and CRA-2026 IS (Table 5, Domski, 2025b)..

	RPPCR		CRA-2026 FS		CRA-2026 IS	
Compound	**Total Quantity (mol)**	**Concentration (M)**	**Total Quantity (mol)**	**Concentration (M)**	**Total Quantity (mol)**	**Concentration (M)**
Acetic acid	5.81×10^5	1.72×10^{-2}	5.40×10^5	5.62×10^{-2}	5.23×10^5	8.29×10^{-2}
Citric acid	6.04×10^4	1.79×10^{-3}	6.08×10^4	6.33×10^{-3}	5.61×10^4	8.88×10^{-3}
EDTA	1.43×10^3	4.22×10^{-5}	1.52×10^3	1.58×10^{-4}	1.34×10^3	2.13×10^{-4}
Oxalic acid	1.95×10^5	5.76×10^{-3}	1.97×10^5	2.05×10^{-2}	1.95×10^5	3.08×10^{-2}

In conclusion, it may be stated that the concentration of the +IV actinides was not affected by the change in the DBR volume because the predominant Th(IV) aqueous species are inorganic hydroxide and hydroxy-carbonate species. The total An(V) concentration is slightly increased by the higher organic ligand concentrations because the Np(V) forms aqueous species with acetate and oxalate while the $NpO2^+$ aqueous species responsible for ~23 – 44% of the dissolved Np(V). Finally, the An(III) total concentration increased because of the increase in the EDTA concentration which forms the dominant Am(III) species $AmEDTA^-$. The results provided herein provide the baseline solubility values for the +III, +IV, and +V actinides for use in the CRA-2026 IS performance assessmsnt calculations.

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APPENDIX A

The Effects of Cementitious Materials on Actinide Solubility for CRA-2026

The EPA submitted "Completeness Questions" to the DOE as part of the CRA-2019 PA. The fifth set of completeness questions (EPA, 2020) included the question *CC5-GEOCHEM-26: Effects of Cements on Brine Chemistry*. The DOE provided responses to this question in two separate Response Packages, response 8 (DOE, 2021a) and response 12, (DOE, 2021b). The DOE's response 12 included an in-depth examination of the effects of cement, as represented by the mineral portlandite, on the actinide baseline solubility values. A similar analysis as was provided in DOE (2021b) is provided here for the 12-panel repository using the minimum volume cases for the GWB and ERDA-6 brines. The difference between the current analysis and that documented in DOE (2021b) is the use of a different thermodynamic database, DATA0.FM6 (Domski, 2023c), the iron and lead reactants, the suppression of calcite, $Am(OH)_3(s)$, and Phase 5, a new DBR volume and repository area, and an updated inventory. These changes are documented in the previous sections of this report, and summarized below.

For the present exercise the following inputs/constraints were implemented, these are the same as those in Section 2 above.

- Volume case: minimum brine volume – the 1x volume case for the CRA-2026 IS will be used;
- Brine types: both ERDA-6 and GWB;
- Conceptual model: reaction path model where minerals initially present in the repository are titrated into a brine and the final equilibrium state achieved through a series of intermediate reaction steps. Both the intensive properties (pH, alkalinity, pCO_2, etc.) and the extensive properties (mass and volume of solution, solvent, and solutes) of the modeled systems are calculated and not set or constrained in the simulations.
- Calcite is suppressed and aragonite is allowed to precipitate when $SI_{aragonite} > 0.0$
- For the simulations anhydrite, halite, brucite, hydromagnesite5424, hibbingite, hydrocerrusite, and portlandite will be used as the reactants. The mass of the portlandite reactant will be scaled to reflect the CRA-2026 IS inventory, and to the mass/volume constraints of EQ3/6.
- $Am(OH)_3(s)$ will be suppressed, and the most stable Am(III), Th(IV) and Np(V) solid phases will be allowed to precipitate to equilibrium.
- Phase 5 will be suppressed.
- The thermodynamic database DATA0.FM6 will be used for the EQ6 calculations.
- It was assumed that 67% of the total cement mass was present as CaO, and that 100% of the CaO can be represented as Portlandite [$Ca(OH)_2(s)$].

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Inputs

The required EQ6 input information is included in the PAIR of Van Soest (2025a and b), in Table 5-6 of the respective PAIR documents. The total mass of cement in Table A-1 is the sum of the reacted and unreacted cement. It was assumed that 67% of the total mass of cement was comprised of CaO and that 100% of the CaO was present as portlandite ($Ca(OH)_2$), this is a conservative assumption as portlandite is more basic than other Ca-SiO_2 cement phases which comprise the majority of the CaO budget. The EQ6 input values for portlandite were scaled to the total dissolved solids (TDS) of the brines, the brine density, and EQ3/6 solvent mass. The values in Table A-1 are calculated in *AP153_Scaling of Solids_CRA_2026-IS.xlsx*, which is provided with this records package.

Note that only the EQ6 input files for the minimum volume, 1x volume cases for GWB and ERDA-6, needed to be edited to include the additional portlandite reactant. It was not necessary to re-run the EQ3NR input files because no new elements were added to the simulation with the addition of portlandite as a reactant.

Table A-1. The EQ6 input values for Portlandite based on the amount of cement in the repository. The values included in this table originate in Table 5-6 in the PAIR documents of Van Soest (2025 a and b).

Calculation of Total moles of Portlandite		
	CRA-2026 IS	**CRA-2026 FS**
Total Mass Cement (kg)	8.55E+06	8.61E+06
Assumed % CaO in Portland Cement	67%	67%
Mass CaO (kg)	5.73E+06	5.77E+06
Mols of CaO	1.02E+08	1.03E+08
portlandite:CaO mol wgt ratio	1.32	1.32
EQ6 Inputs:	**GWB**	
Scaled mols CaO	18.60	12.22
Scaled mols $Ca(OH)_2$	24.57	16.15
EQ6 Inputs:	**ERDA-6**	
Scaled mols CaO	18.18	11.95
Scaled mols $Ca(OH)_2$	24.02	15.79

A – From Table 5 Domski (2025a)

The EQ6 CRA-2026 IS GWB and ERDA-6 1x volume input files were edited to include the portlandite reactant (Table A-1). The input files were run using the DATA0.FM6 thermodynamic database, and the output were post-processed, and the results are tabulated in the following section. The CRA-2026 FS case was not investigated because the interim state case has a smaller DBR volume than the final case, and therefore has higher organic ligand concentrations and a greater amount of portlandite. Thus, the interim state case is more conservative and the final state results would be covered by the interim state results.

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Results

The equilibrium EQ6 solution properties for GWB and ERDA-6 for the baseline and cement (Portlandite) cases are presented in Tables A-2 and A-3.

Table A-2. Equilibrium solution properties for the GWB brine in equilibrium with important solid materials in the repository for the minimum volume (1x volume) case for the baseline case and the baseline case including the cement mineral portlandite.

Condition	No Portlandite	Portlandite
Chemical Entity (M)[A] / Filename	gwb_1x.6o	gwb_cem.6o
B(III)(aq)	0.188	0.114
Na(I)(aq)	4.31	4.38
Mg(II)(aq)	0.932	0.710
K(I)(aq)	0.554	0.336
Ca(II)(aq)	0.013	0.031
Fe(II)(aq)	1.50E-04	1.13E-04
S(VI)(aq)	2.41E-01	7.44E-02
Cl(-I)(aq)	4.75	5.13
Br(-I)(aq)	0.0316	0.0191
Pb(II)(aq)	1.12E-02	1.05E-02
Th(IV)(aq)	5.34E-08	5.41E-08
Np(V)(aq)	9.75E-07	1.13E-06
Am(III)(aq)	1.45E-05	7.87E-06
f_{CO2} (atm)	2.02E-06	2.02E-06
I (m)	8.08	7.33
pH[B]	8.76	8.73
pcH	9.34	9.36
RH (%)[C]	73.0%	73.7%
TIC[D]	2.34E-04	2.36E-04
Mass of Water (kg)	0.734	1.22
molality:Molarity[E]	1.15	1.14

A – All concentrations in molarity (M) unless otherwise specified.
B – Pitzer pH
C – RH = relative humidity. The value of the RH divided by 100 yields the value of the activity of H_2O
D – Total inorganic carbon as HCO_3^-

Table A-3. Equilibrium solution properties for the ERDA-6 brine in equilibrium with important solid materials in the repository for the minimum volume (1x volume) case for the baseline case and the baseline case including the cement mineral portlandite.

Condition	No Portlandite	Portlandite

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Chemical Entity (M)[A] / Filename	erda_1x.6o	erda_cem.6o
B(III)(aq)	0.062	0.042
Na(I)(aq)	4.93	5.09
Mg(II)(aq)	0.546	0.368
K(I)(aq)	0.096	0.065
Ca(II)(aq)	0.013	0.016
Fe(II)(aq)	1.72E-04	1.45E-04
S(VI)(aq)	1.98E-01	1.40E-01
Cl(-I)(aq)	4.86	5.04
Br(-I)(aq)	0.0109	0.0073
Pb(II)(aq)	6.51E-03	4.77E-03
Th(IV)(aq)	5.63E-08	5.78E-08
Np(V)(aq)	4.01E-06	4.09E-06
Am(III)(aq)	1.44E-05	1.05E-05
f_{CO2} (atm)	2.02E-06	2.02E-06
I (m)	7.24	6.91
pH[B]	8.80	8.84
pcH	9.41	9.48
RH (%)[C]	74.2%	74.6%
TIC[D]	2.42E-04	2.52E-04
Mass of Water (kg)	0.892	1.32
molality:Molarity[E]	1.14	1.13

A – All concentrations in molarity (M) unless otherwise specified.
B – Pitzer pH
C – RH = relative humidity. The value of the RH divided by 100 yields the value of the activity of H_2O
D – Total inorganic carbon as HCO_3^-

Tables A-4 and A-5 provide the solids, reactant and products phase, budget data for the GWB and ERDA-6 brines comparing the baseline solubility 1x volume cases with the case which included cement, i.e., portlandite, effects.

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TableA-4. Solid budgets for the reactant and product phases at the initiation of Step 2 and for the final equilibrium for GWB brine with the repository solids. Note: Positive values of delta mass indicate precipitation, and negative indicate dissolution.

	No Portlandite			Portlandite		
Reactants	**Initial Moles**	**Final Moles**	**Delta Moles**	**Initial Moles**	**Final Moles**	**Delta Moles**
Halite	12300.00	12300.00	0.00	12300.00	12297.00	-3.00
Anhydrite	585.00	584.97	-3.00E-02	585.00	585.07	7.00E-02
Brucite	125.00	121.92	-3.08	125.00	153.60	28.60
Hydromagnesite5424	25.10	24.98	-1.17E-01	25.10	18.87	-6.23
Hibbingite	65.40	65.40	0.00	65.40	65.40	0.00
Hydrocerussite	0.57	0.57	-3.16E-03	0.57	0.57	-4.86E-03
Portlandite	NA	NA	NA	24.57	0.00	-2.46E+01
Products	**Initial Moles**	**Final Moles**	**Delta Moles**	**Initial Moles**	**Final Moles**	**Delta Moles**
Phase_3	0.00	1.95	1.95	0.00	1.28	1.28
Whewellite	0.00	0.03	2.96E-02	0.00	0.03	3.02E-02
Aragonite	NA	NA	NA	0.00	24.44	24.44
AmOHCO3(c)	1.60E-02	4.91E-01	4.75E-01	1.60E-02	4.91E-01	4.75E-01
ThO2(am)	2.89E-08	3.84E-08	9.47E-09	2.89E-08	8.13E-09	-2.08E-08
KNpO2CO3	0.00	1.19E-05	1.19E-05	0.00E+00	1.12E-05	1.12E-05

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TableA-5. Solid budgets for the reactant and product phases at the initiation of Step 2 and for the final equilibrium for ERDA-6 brine with the repository solids. Note: Positive values of delta mass indicate precipitation, and negative indicate dissolution.

	No Portlandite			Portlandite		
Reactants	**Initial Moles**	**Final Moles**	**Delta Moles**	**Initial Moles**	**Final Moles**	**Delta Moles**
Halite	12000.00	12000.00	0.00	12000.00	11997.00	-3.00
Anhydrite	572.00	571.97	-3.00E-02	572.00	571.96	-4.00E-02
Brucite	123.00	122.89	-1.10E-01	123.00	152.92	2.99E+01
Hydromagnesite5424	24.50	24.41	-8.60E-02	24.50	18.41	-6.09E+00
Hibbingite	63.90	63.90	0.00	63.90	63.90	0.00
Hydrocerussite	0.56	0.55	-2.20E-03	0.56	0.55	-2.39E-03
Portlandite	NA	NA	NA	2.40E+01	0.00	-2.40E+01
Products	**Initial Moles**	**Final Moles**	**Delta Moles**	**Initial Moles**	**Final Moles**	**Delta Moles**
Whewellite	0.00	3.00E-02	3.00E-02	0.00	3.02E-02	3.02E-02
Aragonite	NA	NA	NA	0.00E+00	2.40E+01	2.40E+01
AmOHCO3(c)	1.60E-02	3.62E-01	3.46E-01	1.60E-02	3.62E-01	3.46E-01
ThO2(am)	0.00	6.66E-08	6.66E-08	0.00	3.70E-08	3.70E-08
KNpO2CO3	0.00	2.29E-05	2.29E-05	0.00	2.08E-05	2.08E-05

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Discussion and Conclusions

The EQ6 results show that the effects of cement, represented as portlandite, are neutralized by the MgO buffer. The Ca^{2+} from the dissolution of portlandite and the CO_3^{2-} from the dissolution of hydromagnesite results in the formation of a calcium carbonate phase, aragonite in this case, while the hydroxide from the portlandite combines with H^+ ion to form water via the reaction:

$$4\,\mathrm{Ca(OH)_2} + Mg_5(CO_3)_4(OH)_2 * 4\,H_2O + 10\,H^+ \rightleftharpoons 4\,CaCO_3 + 5\,Mg^{2+} + 14\,H_2O \quad (Eq\ A-1)$$

The reaction, equation A-1, shows that four moles of portlandite are neutralized per mole of hydromagnesite which releases 5 moles of Mg^{2+} while forming 4 moles of $CaCO_3$ and 14 moles of water.. This exercise demonstrates that there is sufficient MgO buffer to neutralize the potential pH increase caused by cement (portlandite) dissolution. Tables A-4 and A-5 show that the moles of hydromagnesite consumed in the cement cases is ¼ of the moles of portlandite which is consistent with the stoichiometry of Equation A-1, and sufficient to maintain the system pH at a value consistent with the minimum solubility of the actinide phases. The negligible increase in the pH for the cement cases was caused by the increased value of water activity from the reaction between hydromagnesite and portlandite (Equation A-1).

The small changes observed in the actinide concentrations for the cement cases can be attributed to the effects of the increased water activity due to liberation of 14 moles of water per mole of hydromagnesite consumed from portlandite dissolution. This additional water had two effects: 1) The increased activity of water slightly increased the solution pH, i.e., increased the hydroxide, OH^-, concentration; and 2) the greater mass of water caused dilution effects of conservative species, such as the organic ligands. The Am(III) concentration saw the greatest change dropping by 46% in GWB and 27% in ERDA-6. This decrease was caused by dilution of the EDTA concentration, thus decreasing the $AmEDTA^-$ concentration, from the increased water mass. While the Th(IV) concentrations increased by 1.4% for GWB and 2.5% for ERDA-6; negligible values caused by the slight increase in the OH^- concentration which increased the primary thorium species ThO_4(aq). The Np(V) concentration showed a slight increase for the cement cases, where in GWB it increased by 15.6% and 2.1% in ERDA-6. The changes can be attributed to a drop in the $MgAcetate^+$ concentration caused by dilution of acetate which acted to alter the equilibrium and increase the NpO_2Acetate(aq) concentration. The effect is less pronounced in the ERDA-6 brine because it has a lower, by ~50%, Mg^{2+} concentration than the GWB.

Portland cement consists primarily of calcium, silica, aluminum, iron, magnesium, and sulfur. The phases which comprise cured Portland cement are a suite of complex solids which include portlandite. While portlandite may be a reasonable analog to test the pH effects of cement on the WIPP system it is unknown if the dissolution of actual Portland cement would contribute as much water to the system as pure portlandite. Therefore, the results of increasing the mass of water in the system should be considered uncertain.

Similar to the solution compositions results the solid inventory results shown in Tables A-3 and A-4 provide further support that the MgO buffer provides sufficient capacity to neutralize the effects of cement on the actinide solubilities. For both GWB and ERDA-6 an additional ~6 moles of hydromagnesite was consumed in the cement case versus the baseline case, this corresponds to

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¼ of the portlandite budget because 1 mole of hydromagnesite neutralizes 4 moles of portlandite. Should the hydromagnesite budget be less than 25% of the portlandite budget, on a mole basis, then there could be deleterious effects on the actinide solubility values and further investigation may be required.

For CRA-2026 the effects of cementitious materials on the solubility of the +III, +IV, and +V actinides may be discounted as insignificant and do not need to be included in PA calculation. The difference between the current analysis and that documented in DOE (2021b) is the use of a different thermodynamic database, DATA0.FM6 (Domski, 2023c), the iron and lead reactants, the suppression of calcite, $Am(OH)_3(s)$, and Phase 5, a new DBR volume and repository area, and an updated inventory. These changes had a negligible effect on the dissolved actinide concentrations, and therefore, do not need to be accounted for in the CRA-2026 PA.

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