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Waste Isolation Pilot Plant

Prediction of Baseline Actinide Solubilities for the WIPP CRA-2014 PA

Work Carried Out under Task 3 of the Analysis Plan for WIPP Near-Field Geochemical Process Modeling, AP 153, Rev. 1.
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1 INTRODUCTION

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. 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 element and WIPP brine under expected near-field chemical conditions. However, PA codes actually use actinide solubilities that are the products of the baseline solubilities and sampled uncertainty factors that describe possible deviations of the predicted Th(IV) and Am(III) solubilities from experimentally measured solubilities. The reason for using these uncertainty factors is to adjust the baseline solubilities up if the model underpredicts the experimentally measured solubilities, or to adjust the baseline solubilities down if the model overpredicts the measured solubilities. New uncertainty factors are being established in a separate analysis.

The two standard WIPP brines used in this analysis 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.

This analysis does not provide any solubilities for U(VI) because a thermodynamic speciation-and-solubility model has not been developed for U(VI). Instead, the EPA specified that an estimate of 1×10^{-3} M be used for the solubility of U(VI) in GWB and ERDA-6. This estimate has been used beginning with the CRA-2004 PABC. Furthermore, the EPA specified a fixed value for its estimate of the solubility of U(VI) in GWB and ERDA-6 (U.S. EPA, 2006).

This analysis report also provides the compositions of these brines and the values of parameters such as f_{CO_2}, pH, pcH, and TIC. The parameter f_{CO_2} is the fugacity of carbon dioxide (CO_2), which is similar to its partial pressure, in the brines. The pH is the negative, common logarithm of the activity of H^+. The pcH is the negative, common logarithm of the molar concentration of H^+. Finally, TIC is the total inorganic carbon concentration of the brines.

SNL PA personnel will use these baseline solubilities for Th(IV), Np(V), and Am(III) in the PA for the third recertification of the WIPP by the U.S. Environmental Protection Agency (EPA) (the 2014 Compliance Recertification Application, or CRA-2014 PA). This PA will use solubilities that depend on the volume of brine released from the repository.

We used EQ3/6, Version 8.0a, (Wolery and Jarek, 2003; Wolery, 2008; Wolery et al., 2010; Xiong, 2011b) and the thermodynamic database (DB) DATA0.FMT.R2, also known as

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DATA0.FM1 (Xiong, 2011a) for this analysis. Wolery (2008), Wolery et al. (2010) and Xiong (2011b) completed the qualification of Version 8.0a of EQ3/6 according to Sandia National Laboratories' (SNL's) WIPP quality assurance (QA) procedures for WIPP compliance-related actinide-solubility calculations.

We carried out this analysis under Task 5 of AP-153, Rev. 1, the current analysis plan (AP) for WIPP near-field geochemical process modeling (Brush et al., 2012a, Subsection 4.5). AP-153, Rev. 1, describes the modeling to be carried out from the completion of the Performance Assessment Baseline Calculations (PABC) for the second WIPP Compliance Recertification Application (CRA-2009-PABC) through the CRA-2014 PABC, if the EPA requires another PABC.

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 +II 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 $CaCO_3$
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
DB	(thermodynamic) database

Table 1 continued on next page

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

Abbreviation, Acronym, or Initialism	Definition
CRA-2004	the first WIPP Compliance Recertification Application, submitted to the EPA in March 2005
CRA-2009	the second WIPP Compliance Recertification Application, submitted to the EPA in March 2009
CRA-2014	the third WIPP Compliance Recertification Application, to be submitted to the EPA in March 2014
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)
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 $I = \frac{1}{2} \times \Sigma_i(M_i \times z_i^2)$, 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)
M	molar

Table 1 continued on next page

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

Abbreviation, Acronym, or Initialism	Definition
m	meters or molal
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
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
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
WIPP	Waste Isolation Pilot Plant
wt %	weight percent

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2 METHODS

The objective of this analysis was to provide the solubilities of the actinide elements Th(IV), Np(V), and Am(III) in the standard WIPP brines GWB and ERDA-6 as a function of the volume of these brines in the repository. This report also provides the predicted compositions of GWB and ERDA-6 after equilibration with the important solids in the repository. Brush et al. (2012a) described the methods used to calculate the solubilities of Th(IV), Np(V), and Am(III) 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 Brush et al. (2012b).

We used 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 × 17,400 m^3 (Brush and Domski, 2012). Table 2 (see next page) 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 thus increase their solubilities. A volume of 17,400 m^3 is the minimum volume of brine required for a direct brine release (DBR) from the repository (Clayton, 2008). A DBR is defined as a release of brine that could occur directly from the repository to the surface above the repository (i.e., without lateral transport through an offsite transport pathway such as the Culebra Member of the Rustler Fm.). Brush and Domski (2012) used factors of 1, 2, 3, 4, or 5 at the request of WIPP PA personnel, who determined that all of the DBRs in the CRA 2009 PABC had volumes that varied between 1 and 5 × the minimum volume of 17,400 m^3. Brush and Domski (2012) calculated the concentrations of acetate, citrate, EDTA, and oxalate in 1 ×, 2 ×, 3 ×, 4 ×, and 5 × 17,400 $m^3$of brine by assuming that the total masses of these organic ligands in the waste would dissolve completely in these volumes of brine.

We used EQ3/6, Version 8.0a (Wolery and Jarek, 2003; Wolery, 2008; Wolery et al., 2010) 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: (1) acetate, citrate, EDTA, and oxalate; and (2) ThO_2(am), $KNpO_2CO_3$, and $Am(OH)_3$(s)), the solids most likely to control the solubilities of Th(IV), Am(III), and Np(V) in the repository (Brush et al., 2012a). In step 2, we reacted these brines 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., 2012a) and predicted the solubilities of Th(IV), Np(V), and Am(III) and the compositions of GWB and ERDA-6 after equilibration with the important solids. 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 — especially 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 f_{CO_2}, pH, pcH, TIC.

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Table 2. Dissolved Concentrations of Organic Ligands (M) in the Minimum Volume of Brine 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	2.30×10^{-2}	1.15×10^{-2}	7.68×10^{-3}	5.76×10^{-3}	4.61×10^{-3}
Citrate	2.33×10^{-3}	1.16×10^{-3}	7.76×10^{-4}	5.82×10^{-4}	4.65×10^{-4}
EDTA	7.40×10^{-5}	3.70×10^{-5}	2.47×10^{-5}	1.85×10^{-5}	1.48×10^{-5}
Oxalate	1.18×10^{-2}	5.90×10^{-3}	3.93×10^{-3}	2.95×10^{-3}	2.36×10^{-3}

For step 1, we used the speciation and solubility code EQ3NR to add the organic ligands and the actinide-bearing solids to GWB and ERDA-6. We set the initial concentrations of acetate, citrate, EDTA, and oxalate equal to those in volumes of GWB and ERDA-6 that are 1 ×, 2 ×, 3 ×, 4 ×, and 5 × 17,400 m^3. We set the initial value of the total inorganic carbon (TIC) concentrations of both brines 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) we 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 the rest of the calculations). The code charge balanced on H^+; speciated all of the dissolved elements; and calculated the values of parameters such as f_{CO_2}, pH, and TIC. The code also wrote a "pickup" file (*.3p file) for step 2. The *.3p file is called a pickup file because it is copied and pasted into an EQ6 input file, and provides all of the information on the solution and solids required for the next EQ6 run (see below).

For step 2, we used the reaction-path code EQ6 to titrate the solids halite (NaCl), anhydrite ($CaSO_4$), brucite, and hydromagnesite into GWB and ERDA-6. We used halite and anhydrite to simulate the most important minerals in the Salado Fm. at or near the stratigraphic horizon of the repository; and brucite and hydromagnesite to simulate the expected hydration and carbonation products, respectively, of MgO (the WIPP engineered barrier). As EQ6 titrated in these solids, halite and anhydrite dissolved until the brine became saturated with these solids (i.e., until the concentrations of Na^+, Cl^-, Ca^{2+}, and SO_4^{2-} reached their solubility limits). The reaction then continued until brucite and hydromagnesite equilibrated with GWB (i.e., until GWB reached its invariant point). EQ6 then calculated the moles of solids that dissolved and/or precipitated, speciated all of the dissolved elements; and recalculated the values of parameters such as f_{CO_2}, pcH, TIC, etc.

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Brush et al. (2011) used a slightly different procedure for ERDA-6. First, they used EQ6 to titrate just halite and anhydrite into the brine (step 2a). During this step, they titrated halite and anhydrite into ERDA-6 until this brine became saturated with these solids (i.e., until Na^+, Cl^-, Ca^{2+}, and SO_4^{2-} reached their solubility limits). At the end of step 2a, EQ6 wrote a pickup file (*.6p file), which provided all of the information on the solution and solids required for step 2b. During step 2b, they titrated in brucite and hydromagnesite as ERDA-6 remained saturated with halite and anhydrite. The reaction continued until brucite and hydromagnesite equilibrated with ERDA-6 (i.e., until this brine reached its invariant point). EQ6 then calculated the moles of solids that dissolved and/or precipitated, speciated all of the dissolved elements; and recalculated the values of parameters such as f_{CO_2}, pcH, TIC, etc. Because Brush et al. (2012a, Subsection 4.3) anticipated using steps 2a and 2b for this analysis, combination of these two steps into step 2 for this analysis was a deviation from AP-153, Rev. 1.

Table 3 summarizes these EQ3/6 calculations for GWB and ERDA-6.

Table 3. Summary of EQ3/6 Calculations Carried Out with GWB and ERDA-6 for this Analysis.

Description of Step	GWB	ERDA-6
1	Used EQ3NR to add organic ligands and actinide-bearing solids	Used EQ3NR to add organic ligands and actinide-bearing solids
2	Used EQ6 to titrate in halite, anhydrite, brucite, and hydromagnesite	Used EQ6 to titrate in halite, anhydrite, brucite, and hydromagnesite

For step 2, we used quantities of brine, halite, anhydrite, brucite, and hydromagnesite similar to those that 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 17,400 m^3 of brine to 1 kg of water. EQ3/6 allows the user to specify the composition and specific gravity of the aqueous phase present at the start of a run. However, the code assumes that exactly 1 kg of H_2O is present in the solution and uses the specific gravity entered by the user to calculate the volume of solution. We used spreadsheet calculations to scale down (1) the quantities of halite and anhydrite present in the disturbed rock zone (DRZ) surrounding the repository, and (2) the quantity of MgO that will be emplaced in the repository. The spreadsheet, entitled "AP-153_Tasks 1 and 2, Scaling of Solids.xls" is in the zip file AP153Task1Data.zip in library LIBEQ36, class AP153, in the Sandia/WIPP software Configuration Management System (CMS). Table 4 (see next page) provides the locations of this and the other files used for our EQ3/6 calculations. To calculate the quantities of halite and anhydrite, we used the conservatively large DRZ currently implemented in WIPP PA and the assumption that the DRZ comprises 90 wt % halite and 10 wt % anhydrite. This mineralogical composition

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is similar to Brush's (1990) interpretation of the results of Stein's (1985) mineralogical analysis of the Salado Fm. at or near the stratigraphic horizon of the repository: Brush (1990) concluded that, for use in geochemical modeling, the Salado consists of 93.2 wt % halite and 1.7 wt % each of anhydrite, gypsum ($CaSO_4 \cdot 2H_2O$), magnesite ($MgCO_3$), and polyhalite ($K_2MgCa_2(SO_4)_4 \cdot 2H_2O$). However, we assumed for this analysis that the Salado contains 90 wt % halite and 10 wt % anhydrite because the conceptual models for WIPP near-field chemistry include only halite and anhydrite (SCA, 2008). For run 1, we also assumed that the MgO that will be emplaced in the repository will be present half as brucite and half as hydromagnesite; this assumption ensured that ample CO_2 was present without having to use a microbial reaction to titrate in CO_2.

Table 4. 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_Tasks 1 and 2, Scaling of Solids.xls	In zip file AP153Task1Data.zip, library LIBEQ36, class AP153
EQ3/6 DB DATA0.FMT.R2 also called DATA0.FM1	In zip file DATA0_FMT.ZIP, library LIBEQ36, class DATABASES
Excel macro GetEQData.xls	In zip file AP153Rev1Task3Data.zip, library LIBEQ36, class AP153
EQ3/6 I/O files and Excel spreadsheets with extracted data	In zip file AP153Rev1Task3IOfilesData.zip, library LIBEQ36, class AP153

We used EQ6 in closed-system mode (model variable IOPT1 = 0) for step 2. Closed-system mode consists of the simulated titration (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. We suppressed (prevented from precipitating) the solids aragonite ($CaCO_3$), calcite ($CaCO_3$), dolomite ($CaMg(CO_3)_2$), hydromagnesite with the composition $Mg_4(CO_3)_3(OH)_2 \cdot 3H_2O$, and nesquehonite ($MgCO_3 \cdot 3H_2O$) throughout step 2. We suppressed these phases to ensure that this analysis was consistent with the near-field chemical conceptual models (SCA, 2008; Brush et al., 2012a).

Paul Domski carried out all of the EQ3/6 runs described above under the WIPP PA run-control system.

We used the EQ3/6 DB DATA0.FM1 (Xiong, 2011a) for this analysis. Brush et al. (2012a, Subsection 2.2.4) described the history of all DBs used for previous

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WIPP compliance-related actinide-solubility calculations, and discuss the difference between the DBs used by Brush et al. (2011) and the DB used for this analysis.

We extracted the output from these EQ6 *.6o files by running the Excel macro "GetEQData.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.xls, and the Excel spreadsheets that contain the output extracted with GetEQData.xls are in zip file AP153Rev1Task3Data.zip in library LIBEQ36, class AP153, in the CMS.

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3 RESULTS

Table 5 (see next page) 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 × 17,400 m^3, the minimum volume of brine required for a direct brine release (DBR) from the repository (Clayton, 2008). Table 6 provides comparable information for ERDA-6. Brush et al. (2012a, 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 C content of the brines.

Table 7 shows the dissolved species distributions predicted for Th(IV) in the minimum volume and 5 × the minimum volume of GWB. Table 8 shows the species distributions for Th(IV) in the minimum volume and 5 × the minimum volume of ERDA-6 . Tables 9, 10, 11, and 12 provide comparable information for Np(V) and Am(III).

Table 13 compares the solubilities of Th(IV), Np(V), and Am(III) predicted for the minimum brine volume of 17,400 m^3 for the CRA-2014 PA with those predicted for the CCA PA, the PAVT, and the CRA-2004 PA. Table 13 also compares the values of f_{CO_2} and pH predicted for these compliance-related calculations.

Comparison of these results is not straightforward because several assumptions or other factors changed from calculation to calculation. These include: (1) assumptions as to which carbonation reaction will buffer f_{CO_2} (i.e., brucite-magnesite or brucite-hydromagnesite; see Brush and Xiong, 2012a, Subsection 2.1.2), (2) changes in the concentrations of organic ligands in the brines used to calculate these solubilities (see Table 2 above), and (3) changes in the thermodynamic databases (Brush and Xiong, 2012a, Subsection 2.2.4). Replacement of FMT Babb and Nowak, 1997 and addenda; Wang, 1998) by EQ3/6, Version 8.0a (Wolery and Jarek, 2003; Wolery, 2008; Wolery et al., 2010; Xiong, 2011b) between the CRA-2009 PABC and the CRA-2014 PA did not have any affect on these results.

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Table 5. 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)	0.186	0.186	0.186	0.186	0.186
Na(I)(aq)	4.77	4.78	4.78	4.78	4.78
Mg(II)(aq)	0.330	0.319	0.316	0.314	0.313
K(I)(aq)	0.550	0.549	0.549	0.549	0.549
Ca(II)(aq)	0.0111	0.0112	0.0113	0.0113	0.0113
S(VI)(aq)	0.216	0.209	0.207	0.206	0.205
Cl(-I)(aq)	5.36	5.38	5.39	5.39	5.39
Br(-I)(aq)	0.0313	0.0313	0.0313	0.0313	0.0313
Th(IV)(aq)	6.05×10^{-8}	6.06×10^{-8}	6.07×10^{-8}	6.07×10^{-8}	6.07×10^{-8}
Np(V)(aq)	2.77×10^{-7}	2.18×10^{-7}	1.98×10^{-7}	1.88×10^{-7}	1.82×10^{-7}
Am(III)(aq)	2.59×10^{-6}	1.38×10^{-6}	9.74×10^{-7}	7.69×10^{-7}	6.47×10^{-7}
f_{CO_2} (atm)	3.14×10^{-6}	3.14×10^{-6}	3.14×10^{-6}	3.14×10^{-6}	3.14×10^{-6}
I	6.44	6.42	6.42	6.41	6.41
pH[B]	8.82	8.82	8.82	8.82	8.82
pcH	9.54	9.54	9.54	9.54	9.54
RH (%)[C]	73.5	73.5	73.6	73.6	73.6
TIC[D]	3.79×10^{-4}	3.79×10^{-4}	3.79×10^{-4}	3.79×10^{-4}	3.80×10^{-4}

Footnotes for Table 5 provided on next page.

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Footnotes for Table 5:

A. Based on a minimum brine volume of 17,400 m^3 (Clayton, 2008)
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.

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Table 6. 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)	0.0623	0.0624	0.0624	0.0624	0.0624
Na(I)(aq)	5.30	5.32	5.33	5.33	5.33
Mg(II)(aq)	0.136	0.119	0.114	0.112	0.111
K(I)(aq)	0.0960	0.0960	0.0960	0.0960	0.0960
Ca(II)(aq)	0.0116	0.0119	0.0119	0.0119	0.0119
S(VI)(aq)	0.182	0.174	0.172	0.171	0.171
Cl(-I)(aq)	5.24	5.25	5.26	5.26	5.26
Br(-I)(aq)	0.0109	0.0109	0.0109	0.0109	0.0109
Th(IV)(aq)	7.02×10^{-8}	7.14×10^{-8}	7.17×10^{-8}	7.19×10^{-8}	7.20×10^{-8}
Np(V)(aq)	8.76×10^{-7}	7.39×10^{-7}	6.86×10^{-7}	6.6×10^{-7}	6.44×10^{-7}
Am(III)(aq)	1.48×10^{-6}	8.59×10^{-7}	5.99×10^{-7}	4.69×10^{-7}	3.92×10^{-7}
f_{CO_2} (atm)	3.14×10^{-6}	3.14×10^{-6}	3.14×10^{-6}	3.14×10^{-6}	3.14×10^{-6}
I	5.99	5.96	5.94	5.94	5.94
pH[B]	8.99	9.01	9.02	9.02	9.02
pcH	9.69	9.72	9.72	9.72	9.72
RH (%)[C]	74.7	74.7	74.8	74.8	74.8
TIC[D]	4.55×10^{-4}	4.69×10^{-4}	4.72×10^{-4}	4.74×10^{-4}	4.75×10^{-4}

Footnotes for Table 6 provided on next page.

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Footnotes for Table 6:

A. Based on a minimum brine volume of 17,400 m^3 (Clayton, 2008)
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.

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Table 7. 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
$Th(OH)_4(aq)$	4.55×10^{-8}	75.12	$Th(OH)_4(aq)$	4.56×10^{-8}	75.10
$Th(OH)_3CO_3^-$	1.51×10^{-8}	24.88	$Th(OH)_3CO_3^-$	1.51×10^{-8}	24.90
ThEDTA(aq)	6.29×10^{-17}	-	ThEDTA(aq)	1.26×10^{-17}	-
$Th(CO_3)_5^{6-}$	3.72×10^{-17}	-	$Th(CO_3)_5^{6-}$	2.78×10^{-17}	-
$Th(SO_4)_3^{2-}$	2.10×10^{-18}	-	$Th(SO_4)_3^{2-}$	1.76×10^{-18}	-
$ThCit^+$	8.46×10^{-20}	-	$ThCit^+$	1.69×10^{-20}	-
$Th(SO_4)_2(aq)$	6.07×10^{-20}	-	$Th(SO_4)_2(aq)$	5.28×10^{-20}	-
$ThAc_2^{2+}$	2.84×10^{-20}	-	$ThAc_2^{2+}$	1.08×10^{-21}	-
$ThAc^{3+}$	1.21×10^{-21}	-	$ThAc^{3+}$	2.17×10^{-22}	-
$ThOx^{2+}$	3.17×10^{-23}	-	$ThOx^{2+}$	2.85×10^{-23}	-
Th^{4+}	3.45×10^{-25}	-	Th^{4+}	3.01×10^{-25}	-
Total	6.05×10^{-8}	100.00	Total	6.07×10^{-8}	100.00

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Table 8. 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
$Th(OH)_4(aq)$	4.75×10^{-8}	67.68	$Th(OH)_4(aq)$	4.76×10^{-8}	66.15
$Th(OH)_3CO_3^-$	2.27×10^{-8}	32.32	$Th(OH)_3CO_3^-$	2.44×10^{-8}	33.85
$Th(CO_3)_5^{6-}$	3.80×10^{-17}	-	$Th(CO_3)_5^{6-}$	3.63×10^{-17}	-
ThEDTA(aq)	2.66×10^{-17}	-	ThEDTA(aq)	5.37×10^{-18}	-
$Th(SO_4)_3^{2-}$	5.03×10^{-19}	-	$Th(SO_4)_3^{2-}$	3.00×10^{-19}	-
$ThCit^+$	8.86×10^{-20}	-	$ThCit^+$	1.51×10^{-20}	-
$Th(SO_4)_2(aq)$	9.64×10^{-21}	-	$Th(SO_4)_2(aq)$	6.15×10^{-21}	-
$ThAc_2^{2+}$	7.18×10^{-21}	-	$ThAc_2^{2+}$	3.20×10^{-22}	-
$ThAc^{3+}$	3.29×10^{-22}	-	$ThAc^{3+}$	5.60×10^{-23}	-
$ThOx^{2+}$	1.50×10^{-23}	-	$ThOx^{2+}$	1.02×10^{-23}	-
Th^{4+}	1.26×10^{-25}	-	Th^{4+}	8.53×10^{-26}	-
Total	7.02×10^{-8}	100.00	Total	7.20×10^{-8}	100.00

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Table 9. 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
$NpO_2Ac(aq)$	1.19×10^{-7}	42.85	$NpO_2Ac(aq)$	2.41×10^{-8}	11.37
$NpO_2CO_3^-$	7.92×10^{-8}	28.58	$NpO_2CO_3^-$	8.06×10^{-8}	45.08
NpO_2^+	5.49×10^{-8}	19.82	NpO_2^+	5.45×10^{-8}	30.51
NpO_2Ox^-	2.00×10^{-8}	7.23	NpO_2Ox^-	1.92×10^{-8}	10.79
$NpO_2(OH)(aq)$	2.66×10^{-9}	0.96	$NpO_2(OH)(aq)$	2.71×10^{-9}	1.51
$NpO_2(CO_3)_2^{3-}$	1.22×10^{-9}	0.44	$NpO_2(CO_3)_2^{3-}$	1.24×10^{-9}	0.69
NpO_2Cit^{2-}	3.43×10^{-10}	0.12	NpO_2Cit^{2-}	6.92×10^{-11}	0.04
$NpO_2(CO_3)_3^{5-}$	1.12×10^{-11}	-	$NpO_2(CO_3)_3^{5-}$	1.10×10^{-11}	0.01
$NpO_2(OH)_2^-$	5.24×10^{-12}	-	$NpO_2(OH)_2^-$	5.36×10^{-12}	-
NpO_2EDTA^{3-}	1.57×10^{-12}	-	NpO_2EDTA^{3-}	3.08×10^{-13}	-
NpO_2HEDTA^{2-}	5.43×10^{-15}	-	NpO_2HEDTA^{2-}	1.10×10^{-15}	-
$NpO_2H_2EDTA^-$	8.18×10^{-19}	-	$NpO_2H_2EDTA^-$	1.68×10^{-19}	-
Total	2.77×10^{-7}	100.00	Total	1.82×10^{-7}	100.00

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Table 10. 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
$NpO_2CO_3^-$	4.06×10^{-7}	46.28	$NpO_2CO_3^-$	4.06×10^{-7}	62.94
$NpO_2Ac(aq)$	2.57×10^{-7}	29.27	$NpO_2Ac(aq)$	5.54×10^{-8}	8.60
NpO_2^+	1.41×10^{-7}	16.14	NpO_2^+	1.20×10^{-7}	18.70
NpO_2Ox^-	5.00×10^{-8}	5.71	NpO_2Ox^-	4.08×10^{-8}	6.33
$NpO_2(CO_3)_2^{3-}$	1.13×10^{-8}	1.28	$NpO_2(CO_3)_2^{3-}$	1.28×10^{-8}	1.98
$NpO_2(OH)(aq)$	9.37×10^{-9}	1.07	$NpO_2(OH)(aq)$	8.78×10^{-9}	1.36
NpO_2Cit^{2-}	2.02×10^{-9}	0.23	NpO_2Cit^{2-}	3.91×10^{-10}	0.06
$NpO_2(CO_3)_3^{5-}$	1.22×10^{-10}	0.01	$NpO_2(CO_3)_3^{5-}$	1.48×10^{-10}	0.02
$NpO_2(OH)_2^-$	2.65×10^{-11}	-	$NpO_2(OH)_2^-$	2.67×10^{-11}	-
NpO_2EDTA^{3-}	4.05×10^{-12}	-	NpO_2EDTA^{3-}	8.60×10^{-13}	-
NpO_2HEDTA^{2-}	1.83×10^{-14}	-	NpO_2HEDTA^{2-}	3.92×10^{-15}	-
$NpO_2H_2EDTA^-$	3.25×10^{-18}	-	$NpO_2H_2EDTA^-$	6.72×10^{-19}	-
Total	8.76×10^{-7}	99.99	Total	6.44×10^{-7}	99.99

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Table 11. 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 $Am(OH)_3$.

GWB, minimum volume			GWB, 5 × minimum volume		
Am(III) Species	Concentration (M)	Percent of Solubility	Am(III) Species	Concentration (M)	Percent of Solubility
$AmEDTA^-$	2.44×10^{-6}	94.12	$AmEDTA^-$	4.91×10^{-7}	73.46
$Am(OH)_2^+$	1.47×10^{-7}	5.67	$Am(OH)_2^+$	1.52×10^{-7}	26.00
$AmAc^{2+}$	1.62×10^{-9}	0.06	$AmAc^{2+}$	3.18×10^{-10}	0.05
$Am(OH)^{2+}$	1.33×10^{-9}	0.05	$Am(OH)^{2+}$	1.31×10^{-9}	0.22
AmCit(aq)	9.89×10^{-10}	0.04	AmCit(aq)	2.03×10^{-10}	0.04
$Am(OH)_3(aq)$	7.49×10^{-10}	0.03	$Am(OH)_3(aq)$	7.63×10^{-10}	0.13
$AmCO_3^+$	2.62×10^{-10}	0.01	$AmCO_3^+$	2.60×10^{-10}	0.04
$Am(CO_3)_2^-$	2.05×10^{-10}	-	$Am(CO_3)_2^-$	2.06×10^{-10}	0.04
$Am(CO_3)_3^{3-}$	4.83×10^{-11}	-	$Am(CO_3)_3^{3-}$	4.79×10^{-11}	-
$AmSO_4^+$	3.99×10^{-11}	-	$AmSO_4^+$	3.76×10^{-11}	-
$AmOx^+$	7.77×10^{-12}	-	$AmOx^+$	7.45×10^{-12}	-
$Am(SO_4)_2^-$	6.18×10^{-12}	-	$Am(SO_4)_2^-$	5.51×10^{-12}	-
Am^{3+}	5.63×10^{-12}	-	Am^{3+}	5.84×10^{-12}	-
$Am(CO_3)_4^{5-}$	2.23×10^{-12}	-	$Am(CO_3)_4^{5-}$	2.05×10^{-12}	-
$AmCl^{2+}$	6.25×10^{-13}	-	$AmCl^{2+}$	5.84×10^{-13}	-

Table 11 continued on next page.

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Table 11. 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 $Am(OH)_3$ (continued).

GWB, minimum volume			GWB, 5 × minimum volume		
Am(III) Species	Concentration (M)	Percent of Solubility	Am(III) Species	Concentration (M)	Percent of Solubility
$AmCl_2^+$	2.49×10^{-14}	-	$AmCl_2^+$	2.35×10^{-14}	-
Total	2.59×10^{-6}	99.98	Total	6.47×10^{-7}	99.98

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Table 12. 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 $Am(OH)_3$.

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
$AmEDTA^-$	1.39×10^{-6}	93.76	$AmEDTA^-$	3.04×10^{-7}	77.63
$Am(OH)_2^+$	8.97×10^{-8}	6.06	$Am(OH)_2^+$	8.57×10^{-8}	21.86
$Am(OH)_3(aq)$	7.03×10^{-10}	0.05	$Am(OH)_3(aq)$	7.18×10^{-10}	0.18
$Am(OH)^{2+}$	5.91×10^{-10}	0.04	$Am(OH)^{2+}$	5.03×10^{-10}	0.13
$AmCit(aq)^+$	5.60×10^{-10}	0.04	$AmCit(aq)^+$	1.03×10^{-10}	0.03
$Am(CO_3)_2^-$	3.11×10^{-10}	0.02	$Am(CO_3)_2^-$	3.36×10^{-10}	0.09
$AmAc^2$	3.05×10^{-10}	0.02	$AmAc^2$	5.96×10^{-11}	0.02
$AmCO_3^+$	1.84×10^{-10}	0.01	$AmCO_3^+$	1.70×10^{-10}	0.04
$Am(CO_3)_3^{3-}$	9.07×10^{-11}	-	$Am(CO_3)_3^{3-}$	1.07×10^{-10}	0.03
$AmSO_4^+$	1.11×10^{-11}	-	$AmSO_4^+$	8.28×10^{-12}	-
$AmOx^+$	3.03×10^{-12}	-	$AmOx^+$	2.32×10^{-12}	-
Am^{3+}	2.31×10^{-12}	-	Am^{3+}	1.96×10^{-12}	-
$Am(SO_4)_2^-$	1.36×10^{-12}	-	$Am(SO_4)_2^-$	9.54×10^{-13}	-
$Am(CO_3)_4^{5-}$	1.27×10^{-12}	-	$Am(CO_3)_4^{5-}$	1.41×10^{-12}	-
$AmCl^{2+}$	1.76×10^{-13}	-	$AmCl^{2+}$	1.32×10^{-13}	-

Table 12 continued on next page.

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Table 12. Comparisons of Distributions of Dissolved Am(III) Species in the Minimum Volume and 5 × the Minimum Volume of ERDA-6 (continued). 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 $Am(OH)_3$ (continued).

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
$AmCl_2^+$	6.41×10^{-15}	-	$AmCl_2^+$	4.84×10^{-15}	-
Total	1.48×10^{-6}	100.00	Total	3.92×10^{-7}	100.01

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Table 13. Comparison of Actinide Solubilities (M), f_{CO_2} (atm), and pH (Pitzer scale[A]) from These and Previous Compliance-Related Calculations.

Property or Actinide Oxidation State	CCA (SPC, Magnesite, w/o Organics, All Vectors)[B]	CCA (ERDA-6, Magnesite, without Organics, All Vectors)[B]	PAVT (SPC, Hydromagnesite without Organics, All Vectors)[C]	PAVT (ERDA-6, Hydromagnesite, without Organics, All Vectors)[C]	CRA-2004 PA (GWB, Hydromagnesite, with Organics, Microbial Vectors)[D]	CRA-2004 PA (ERDA-6, Hydromagnesite, with Organics, Microbial Vectors)[D]
Th(IV)	4.4×10^{-6}	6.0×10^{-9}	1.3×10^{-8}	4.1×10^{-8}	1.19×10^{-8}	2.47×10^{-8}
Np(V)	2.3×10^{-6}	2.2×10^{-6}	2.4×10^{-7}	4.8×10^{-7}	1.02×10^{-6}	5.08×10^{-6}
Am(III)	5.82×10^{-7}	6.52×10^{-8}	1.2×10^{-7}	1.3×10^{-8}	3.07×10^{-7}	1.69×10^{-7}
f_{CO_2}	1.29×10^{-7}	1.29×10^{-7}	3.16×10^{-6}	3.16×10^{-6}	3.16×10^{-6}	3.16×10^{-6}
pH	8.69	9.24	8.69	9.24	8.69	9.02

A. 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.
B. From Novak et al. (1996) and U.S. DOE (1996, Appendix SOTERM), except that Novak et al. (1996) used molal instead of molar units. U.S. EPA (1998) cited Novak and Moore (1996) as the source of the CCA PA solubilities, but the Am(III) solubilities from Novak and Moore (1996) differ from those in Novak et al. (1996) and U.S. DOE (1996).
C. From Trovato (1997). Novak (1997) also calculated actinide solubilities for the PAVT, but the EPA used the results of its own calculations.
D. From Brush and Xiong (2003a, 2003b, 2003c, 2003d) and U.S. DOE (2004, Appendix SOTERM).
E. Brush and Xiong (2005a, 2005b) and Brush (2005). These solubilities were also used for the CRA-2009 PA calculations.
F. Brush et al. (2009)
G. This report

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Table 13. Comparison of Actinide Solubilities (M), f_{CO_2} (atm), and pH (Pitzer Scale[A]) from These and Previous Compliance-Related Calculations (continued).

Property or Actinide Oxidation State	CRA-2004 PABC (GWB, Hydromagnesite, with Organics, All Vectors)[E]	CRA-2004 PABC (ERDA-6, Hydromagnesite, with Organics, All Vectors)[E]	CRA-2009 PABC (GWB, Hydromagnesite, with Organics, All Vectors)[F]	CRA-2009 PABC (ERDA-6, Hydromagnesite, with Organics, All Vectors)[F]	CRA-2014 PA ($GWB_{min.\ vol.}$, Hydromagnesite, with Organics, All Vectors)[G]	CRA-2014 PA ($ERDA\text{-}6_{min.\ vol.}$, Hydromagnesite, with Organics, All Vectors)[G]
Th(IV)	5.64×10^{-8}	6.79×10^{-8}	5.63×10^{-8}	6.98×10^{-8}	6.05×10^{-8}	7.02×10^{-8}
Np(V)	3.55×10^{-7}	8.24×10^{-7}	3.90×10^{-7}	8.75×10^{-7}	2.77×10^{-7}	8.76×10^{-7}
Am(III)	3.87×10^{-7}	2.88×10^{-7}	1.66×10^{-6}	1.51×10^{-6}	2.59×10^{-6}	1.48×10^{-6}
f_{CO_2}	3.16×10^{-6}	3.16×10^{-6}	3.14×10^{-6}	3.14×10^{-6}	3.14×10^{-6}	3.14×10^{-6}
pH	8.69	8.94	8.69	8.98	8.82	8.99

A. 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.
B. From Novak et al. (1996) and U.S. DOE (1996, Appendix SOTERM), except that Novak et al. (1996) used molal instead of molar units. U.S. EPA (1998) cited Novak and Moore (1996) as the source of the CCA PA solubilities, but the Am(III) solubilities from Novak and Moore (1996) differ from those in Novak et al. (1996) and U.S. DOE (1996).
C. From Trovato (1997). Novak (1997) also calculated actinide solubilities for the PAVT, but the EPA used the results of its own calculations.
D. From Brush and Xiong (2003a, 2003b, 2003c, 2003d) and U.S. DOE (2004, Appendix SOTERM).
E. Brush and Xiong (2005a, 2005b) and Brush (2005). These solubilities were also used for the CRA-2009 PA calculations.
F. Brush et al. (2009)
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4 CONCLUSIONS

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. 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 simulates fluids in brine reservoirs in the Castile Fm. SNL PA personnel will use these baseline actinide solubilities in the PA for the CRA-2014 PA). This PA will use solubilities that depend on the volume of brine released from the repository. We used EQ3/6, Version 8.0a, and DATA0.FM1 for this analysis. Section 2 (see above) describes the methods used for this analysis.

Table 5 (see Section 3 above) 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 × 17,400 m^3, the minimum volume of brine required for a direct brine release (DBR) from the repository (Clayton, 2008). Table 6 provides comparable information for ERDA-6. The brucite-hydromagnesite carbonation reaction will control f_{CO_2} and the TIC content of the brines.

Table 7 (Section 3) shows the dissolved species distributions predicted for Th(IV) in the minimum volume and 5 × the minimum volume of GWB. Table 8 shows the species distributions for Th(IV) in the minimum volume and 5 × the minimum volume of ERDA-6 . Tables 9, 10, 11, and 12 provide comparable information for Np(V) and Am(III).

Table 13 (Section 3) compares the solubilities of Th(IV), Np(V), and Am(III) predicted for the minimum brine volume of 17,400 m^3 for the CRA-2014 PA with those predicted for the CCA PA, the PAVT, and the CRA-2004 PA. Table 13 also compares the values of f_{CO_2} and pH predicted for these compliance-related calculations.

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