Sandia National Laboratories
Waste Isolation Pilot Plant

Calculation of Actinide Solubilities for the WIPP Compliance Recertification Application

BOE 1.3.5.1.2

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1 ABBREVIATIONS, ACRONYMS, AND INITIALISMS

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

Table 1. Abbreviations, Acronyms, and Initialisms.

Abbreviation, Acronym, or Initialism	Definition
acetate ion	$CH_3CO_2^-$
Am	americium
am	amorphous
An(III)	actinide element(s) in the +III oxidation state
An(IV)	actinide element(s) in the +IV oxidation state
An(V)	actinide element(s) in the +V oxidation state
An(VI)	actinide element(s) in the +VI oxidation state
anhydrite	$CaSO_4$
B, $B(OH)_3^x$	boron, boric acid
Br, Br^-	bromine, bromide (ion)
Brine A	a synthetic brine representative of intergranular Salado brines
brucite	$Mg(OH)_2$
C	carbon
Ca, Ca^{2+}	calcium, calcium ion
calcite	$CaCO_3$
citrate ion	$((CO_2H)(CH_2))_2C(CO_2)OH^-$
Cl, Cl^-	chlorine, chloride ion
cm	centimeter(s)
CMS	(Compaq Computer Corp., now a part of the Hewlett-Packard Co.) DECset Code Management System
CO_2	carbon dioxide
CO_3^{2-}	carbonate ion
CRA	(WIPP) Compliance Recertification Application
DOE	(U.S.) Department of Energy
EDTA	ethylenediaminetetraacetate $(CH_2CO_2H)_2N(CH_2)_2N(CH_2CO_2H)(CH_2CO_2)^-$
EPA	(U.S.) Environmental Protection Agency
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

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

Abbreviation, Acronym, or Initialism	Definition
Fm.	Formation
FMT or fmt	Fracture-Matrix Transport, a geochemical speciation and solubility code
g	gram(s)
glauberite	$Na_2Ca(SO_4)_2$
GWB	Generic Weep Brine, a synthetic brine representative of intergranular Salado brines
H or H^+	hydrogen or hydrogen ion
halite	NaCl
HCO_3^-	bicarbonate ion
hydromagnesite	$Mg_4(CO_3)_3(OH)_2 \cdot 3H_2O$ or $Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$
hydromagnesite$_{4323}$	$Mg_4(CO_3)_3(OH)_2 \cdot 3H_2O$
hydromagnesite$_{5424}$	$Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$
I	ionic strength
K, K^+	potassium, potassium ion
L	liter(s)
M	molar
m	molal
magnesite	$MgCO_3$
Mg, Mg^{2+}	magnesium, magnesium ion
mg	milligram(s)
MgO	magnesium oxide, used to refer to the WIPP engineered barrier, which includes periclase as the primary constituent and ~5-10 wt % impurities
mM	millimolar
N	nitrogen
Na or Na^+	sodium, sodium ion
nesquehonite	$MgCO_3 \cdot 3H_2O$
Np	neptunium
O	oxygen
OH^-	hydroxide ion
oxalate	$(CO_2H)(CO_2)^-$
PA	performance assessment
PAVT	(U.S. EPA's WIPP) Performance Assessment Verification Test
periclase	pure, crystalline MgO, the primary constituent of the WIPP engineered barrier

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

Abbreviation, Acronym, or Initialism	Definition
pH	the negative, common logarithm of the activity of H^+
Pu	plutonium
Rev.	Revision
RH	relative humidity
SO_4^{2-}	sulfate ion
Sp gr	specific gravity
TDS	total dissolved solids
Th	thorium
U	uranium
WIPP	(U.S. DOE) Waste Isolation Pilot Plant
wt	weight

2 INTRODUCTION

This analysis report describes the calculation of revised actinide solubilities in Waste-Isolation-Pilot-Plant (WIPP) brines. These solubilities will be used for the performance-assessment (PA) calculations for the U.S. Department of Energy's (DOE's) first WIPP Compliance Recertification Application (CRA). These solubilities will replace the solubilities used for the U.S. Environmental Protection Agency's (EPA's) WIPP Performance Assessment Verification Test (PAVT) in 1997, the solubilities currently in the WIPP Project's technical baseline.

This work was carried out under the third task of the analysis plan for the CRA PA solubility calculations (Brush and Xiong, 2003a, Subsection 7.3, FMT Calculations).

3 OBJECTIVES

The objective of this work was to analyze those Fracture-Matrix-Transport (FMT) calculations (runs) described by Brush and Xiong (2003a, Subsection 7.3, FMT Calculations) that provided the solubilities that will be used directly in the CRA PA calculations.

Table 2 lists all of the FMT runs described by Brush and Xiong (2003a, Subsection 7.3). Sandia National Laboratories (SNL)/WIPP PA personnel executed all of these runs under the WIPP PA run-control system (see Brush and Xiong, 2003a, Section 6, Software Description) and archived them in the SNL/WIPP Code Management System (CMS) library entitled lib_ap098_fmt. The four runs that provided the solubilities that will be used for the CRA PA calculations are ap098_fmt_run012.in, ap098_fmt_run012.inguess, ap098_fmt_run012.out, etc. (hereafter referred to as "Run 12" or "12" in the text and in Table 3); Run 18; Run 22; and Run 28.

Table 3 also shows the FMT runs that provided actinide solubilities that will be used in the CRA PA. For ease of comparison, Table 3 is formatted identically to Tables 6 and 7.

We will analyze the remainder of the thirty runs described by Brush and Xiong (2003a, Subsection 7.4) after the CRA PA calculations. We will also carry out additional analysis of the four runs considered in this report. Analysis of the other runs and the additional analysis of the runs considered herein are not required for the CRA PA; however, the additional work to be conducted after the CRA PA will help us develop a better understanding of the effects of factors and parameters such as brine composition, f_{CO_2}, and the presence of organics on actinide speciation and solubilities.

4 CALCULATION OF SOLUBILITIES FOR THE CRA PA CALCULATIONS

We established revised An(III), An(IV), and An(V) solubilities for the CRA PA calculations by: (1) calculating solubilities for Am(III) and using the results for both Pu(III) and Am(III); (2) calculating solubilities for Th(IV) and using the results for Th(IV), U(IV), Np(IV) and Pu(IV); and (3) calculating solubilities for Np(V) and using the results only for Np(V). The results for Np(V) will be used for Np(V) but not for other actinides in the WIPP because Pu will not persist in significant quantities in the +V oxidation state. Brush and Xiong (2003a, Subsection 5.1, CCA Solubilities; and Subsection 5.2, PAVT Solubilities) provided the justification for this approach. The WIPP Actinide Source Term Program did not establish a solubility model for U(VI); instead, it used literature data to estimate the solubilities of U(VI) in the WIPP (Hobart and Moore, 1996; U.S. DOE, 1996, Appendix SOTERM, SOTERM-27 - SOTERM-28). These estimates will be used for U(VI) but not for other actinides because Np and Pu will not persist in significant quantities in the +VI oxidation state.

We calculated An(III), An(IV), and An(V) solubilities for the CRA PA calculations in GWB and ERDA-6. Brush and Xiong (2003a, Subsection 5.1, CCA Solubilities) provided the justification for using ERDA-6 to simulate brines from the Castile Fm.; Brush and Xiong (2003a, Subsection 5.3.1, Use of GWB) provided the justification for using GWB instead of Brine A to simulate intergranular Salado brines at or near the stratigraphic horizon of the WIPP. However, Snider (2003) revised the composition of GWB slightly from that specified by Brush and Xiong (2003a, Table 4 and Table 5). Table 4 of this report provides the revised composition of GWB used to calculate the CRA PA solubilities.

For each brine, we used the brucite $(Mg(OH)_2)$-calcite $(CaCO_3)$ carbonation reaction to buffer f_{CO_2} for the nonmicrobial PA realizations (vectors), and the brucite-hydromagnesite $(Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O)$ carbonation reaction to buffer f_{CO_2} for the microbial vectors. (Thermodynamic data for hydromagnesite with the compositions $Mg_4(CO_3)_3(OH)_2 \cdot 3H_2O$ and $Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$ are in the FMT database. However, the EPA mandated that hydromagnesite with the composition $Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$ be used in the FMT calculations for the PAVT, not hydromagnesite with the composition $Mg_4(CO_3)_3(OH)_2 \cdot 3H_2O$. Furthermore, recent results from a laboratory study of MgO by Snider and Xiong (2002) at SNL imply that, under a controlled atmosphere consisting of 5% CO_2, hydromagnesite with the composition $Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$ is the dominant carbonation product in both GWB and ERDA-6 by about 91 days.) The brucite dissolution reaction buffered pH in all cases. Brush and Xiong (2003a, Subsection 5.2, PAVT Solubilities; and Subsection 5.3.2, Redefinition of Conditions for PA Vectors without Microbial Activity) provided the justification for the use of these reactions.

Table 2. FMT Runs Completed Prior to the CRA PA Calculations. All runs archived in the CMS in lib_ap098_fmt. Runs that provided solubilities for the CRA PA calculations shown in bold font.

Run ID	Brine	f_{CO_2} Buffer	Organics
ap098_fmt_run001.in, ap098_fmt_run001.inguess, ap098_fmt_run001.out, etc.	Brine A	Brucite-calcite	No
ap098_fmt_run002	Brine A	Brucite-calcite	Yes
ap098_fmt_run003	Brine A	Brucite-magnesite	No
ap098_fmt_run004	Brine A	Brucite-magnesite	Yes
ap098_fmt_run005	Brine A	Brucite-hydromagnesite$_{4323}$[1]	No
ap098_fmt_run006	Brine A	Brucite-hydromagnesite$_{4323}$[1]	Yes
ap098_fmt_run007	Brine A	Brucite-hydromagnesite$_{5424}$[2]	No
ap098_fmt_run008	Brine A	Brucite-hydromagnesite$_{5424}$[2]	Yes
ap098_fmt_run009	Brine A	Brucite-nesquehonite	No
ap098_fmt_run010	Brine A	Brucite-nesquehonite	Yes
ap098_fmt_run011	GWB	Brucite-calcite	No
ap098_fmt_run012	**GWB**	**Brucite-calcite**	**Yes**
ap098_fmt_run013	GWB	Brucite-magnesite	No
ap098_fmt_run014	GWB	Brucite-magnesite	Yes
ap098_fmt_run015	GWB	Brucite-hydromagnesite$_{4323}$[1]	No
ap098_fmt_run016	GWB	Brucite-hydromagnesite$_{4323}$[1]	Yes
ap098_fmt_run017	GWB	Brucite-hydromagnesite$_{5424}$[2]	No
ap098_fmt_run018	**GWB**	**Brucite-hydromagnesite$_{5424}$[2]**	**Yes**
ap098_fmt_run019	GWB	Brucite-nesquehonite	No
ap098_fmt_run020	GWB	Brucite-nesquehonite	Yes
ap098_fmt_run021	ERDA-6	Brucite-calcite	No
ap098_fmt_run022	**ERDA-6**	**Brucite-calcite**	**Yes**
ap098_fmt_run023	ERDA-6	Brucite-magnesite	No
ap098_fmt_run024	ERDA-6	Brucite-magnesite	Yes
ap098_fmt_run025	ERDA-6	Brucite-hydromagnesite$_{4323}$[1]	No
ap098_fmt_run026	ERDA-6	Brucite-hydromagnesite$_{4323}$[1]	Yes
ap098_fmt_run027	ERDA-6	Brucite-hydromagnesite$_{5424}$[2]	No
ap098_fmt_run028	**ERDA-6**	**Brucite-hydromagnesite$_{5424}$[2]**	**Yes**
ap098_fmt_run029	ERDA-6	Brucite-nesquehonite	No
ap098_fmt_run030	ERDA-6	Brucite-nesquehonite	Yes

1. Hydromagnesite$_{4323}$ = $Mg_4(CO_3)_3(OH)_2 \cdot 3H_2O$.
2. Hydromagnesite$_{5424}$ = $Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$.

Table 3. FMT Runs Analyzed Prior to the CRA PA Calculations.

Actinide Oxidation State and Brine	Solubility, PAVT, All Vectors, No Organics	Solubility, CRA PA, Nonmicrobial Vectors, No Organics	Solubility, CRA PA, Nonmicrobial Vectors, Organics	Solubility, CRA PA, Microbial Vectors, No Organics	Solubility, CRA PA, Microbial Vectors, Organics
An(III), Brine A	Calculated previously[1]	Analysis incomplete	Analysis incomplete	Analysis incomplete	Analysis incomplete
An(III), GWB	Not calculated[1]	Analysis incomplete	Analyzed Run 12	Analysis incomplete	Analyzed Run 18
An(III), ERDA-6	Calculated previously[1]	Analysis incomplete	Analyzed Run 22	Analysis incomplete	Analyzed Run 28
An(IV), Brine A	Calculated previously[1]	Analysis incomplete	Analysis incomplete	Analysis incomplete	Analysis incomplete
An(IV), GWB	Not calculated[1]	Analysis incomplete	Analyzed Run 12	Analysis incomplete	Analyzed Run 18
An(IV), ERDA-6	Calculated previously[1]	Analysis incomplete	Analyzed Run 22	Analysis incomplete	Analyzed Run 28
An(V), Brine A	Calculated previously[1]	Analysis incomplete	Analysis incomplete	Analysis incomplete	Analysis incomplete
An(V), GWB	Not calculated[1]	Analysis incomplete	Analyzed Run 12	Analysis incomplete	Analyzed Run 18
An(V), ERDA-6	Calculated previously[1]	Analysis incomplete	Analyzed Run 22	Analysis incomplete	Analyzed Run 28

Table 3. FMT Runs Analyzed Prior to the CRA PA Calculations (cont.).

Actinide Oxidation State and Brine	Solubility, PAVT, All Vectors, No Organics	Solubility, CRA PA, Nonmicrobial Vectors, No Organics	Solubility, CRA PA, Nonmicrobial Vectors, Organics	Solubility, CRA PA, Microbial Vectors, No Organics	Solubility, CRA PA, Microbial Vectors, Organics
An(VI), Brine-A	Estimated previously[2]	See Table 7	See Table 7	See Table 7	See Table 7
An(VI), GWB	Not estimated[2]	See Table 7	See Table 7	See Table 7	See Table 7
An(VI), ERDA-6	Estimated previously[2]	See Table 7	See Table 7	See Table 7	See Table 7

1. From Trovato (1997, Attachment 2), U.S. EPA (1998a, Table 5), U.S. EPA (1998b, Subsection 4.10.4, Tables 4.10-1, 4.10-3 and 4.10-4; and Subsection 12.4, Table 12.4-1), and U.S. EPA (1998c, Subsections 5.26–5.32 and Section 6.0, Table 6.4).
2. Estimated for the CCA PA by Hobart and Moore (1996). See also U.S. DOE, 1996, Appendix SOTERM, SOTERM-27 - SOTERM-28).

Table 4. Compositions of Brine A, GWB, and ERDA-6 Prior to Reaction.

Element or Property	Brine A[1]	GWB[2]	ERDA-6[3]
$B(OH)_3$	20 mM[4]	155 mM	63 mM
Na^+	1.83 M	3.48 M	4.87 M
Mg^{2+}	1.44 M	1.00 M	19 mM
K^+	770 mM	458 mM	97 mM
Ca^{2+}	20 mM	14 mM	12 mM
SO_4^{2-}	40 mM	175 mM	170 mM
Cl^-	5.35 M	5.51 M	4.8 M
Br^-	10 mM	26 mM	11 mM
Total inorganic C (as HCO_3^-)	10 mM	Not reported	16 mM
pH	6.5	Not reported	6.17
Sp gr	1.2	1.2	1.216
TDS	306,000 mg/L	Not reported	330,000 mg/L

1. From Molecke (1983).
2. From Snider (2003).
3. From Popielak (1983).
4. Reported by Molecke (1983) as BO_3^{3-}.

For each brine and carbonation reaction, we included the following organic ligands in the solubility calculations for the CRA PA: acetate ($CH_3CO_2^-$), citrate ($((CO_2H)(CH_2))_2C(CO_2)OH^-$), EDTA (ethylenediaminetetraacetate, $(CH_2CO_2H)_2N(CH_2)_2N(CH_2CO_2H)(CH_2CO_2)^-$), and oxalate ($(CO_2H)(CO_2)^-$). Brush and Xiong (2003b) calculated revised concentrations of these organic ligands in WIPP brines based on information provided by Crawford (2003). Table 5 provides the revised concentrations of these ligands used for the CRA PA solubilities.

Table 5. Concentrations of Ligands for the Solubility Calculations for the CRA PA. From Brush and Xiong (2003b) and Crawford (2003).

Ligand	Concentration (M)
Acetate	5.05×10^{-3}
Citrate	3.83×10^{-4}
EDTA	3.87×10^{-6}
Oxalate	2.16×10^{-2}

5 ANALYSIS OF RESULTS

We analyzed FMT Runs 12, 18, 22, and 28 for this report. These runs provided the solubilities that will be used directly in the CRA PA calculations. We will analyze the rest of the runs listed in Table 2 later. We will also carry out additional analysis of the four runs considered in this report. (The solubilities and other information that we will obtain from the other runs is not required for the CRA PA calculations; instead, the additional analysis to be conducted after the CRA PA will help us develop a better understanding of actinide speciation and solubilities in the WIPP.)

We obtained the solids in equilibrium with GWB and ERDA-6 directly from the table entitled "Table of Concentrations for Batch System" in each of the FMT output files. This table identifies the solids present in the first column ("Species Name") by chemical composition and mineral name or other description (if any) connected by a solid line. The nonradioactive solids in equilibrium with GWB in the run carried out for the nonmicrobial vectors were halite (NaCl), anhydrite ($CaSO_4$), brucite, $Mg_2Cl(OH)_3 \cdot 4H_2O$, and calcite. (Because of the presence of $Mg_2Cl(OH)_3 \cdot 4H_2O$, f_{CO_2} was actually buffered by two reactions, the brucite-calcite and the $Mg_2Cl(OH)_3 \cdot 4H_2O$-calcite carbonation reactions; and pH was buffered by two reactions, the brucite and the $Mg_2Cl(OH)_3 \cdot 4H_2O$ dissolution reactions.) The stable solids in equilibrium with GWB in the run for the microbial vectors were halite, anhydrite, brucite, $Mg_2Cl(OH)_3 \cdot 4H_2O$, and hydromagnesite ($Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$). (In this run, f_{CO_2} was actually buffered by two reactions, the brucite-hydromagnesite ($Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$) and the $Mg_2Cl(OH)_3 \cdot 4H_2O$-hydromagnesite carbonation reactions; and pH was buffered by two reactions, the brucite and the $Mg_2Cl(OH)_3 \cdot 4H_2O$ dissolution reactions.) The nonradioactive solids in equilibrium with ERDA-6 in the run conducted for the nonmicrobial vectors were halite, anhydrite, glauberite ($Na_2Ca(SO_4)_2$), brucite, and calcite. Those in equilibrium with ERDA-6 in the run for the microbial vectors were halite, anhydrite, brucite, and hydromagnesite ($Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$). The solids that controlled the solubilities of Th, Np, and Am were $ThO_2(am)$ ("hydrous thorium oxide"), $KNpO_2CO_3$, and $Am(OH)_3$, respectively.

We obtained the density, log f_{CO_2}, ionic strength (I), pH, and relative humidity (RH) of GWB and ERDA-6 at equilibrium with the MgO reaction products from output below "Table of Concentrations for Batch System." Table 6 provides the results for Runs 12, 18, 22, and 28. The RH of these brines is simply related to the activity of H_2O: for example, a RH of 73.3%, calculated for GWB under conditions relevant for the nonmicrobial vectors (brucite-calcite carbonation reaction) with organics (see Table 6), is equivalent to an H_2O activity of 0.733. None of these properties will be used in the CRA PA calculations.

Downes (2003) obtained the solubilities of Th, Np, and Am from Runs 12, 18, 22, and 28 (the solubilities that will be used directly in the CRA PA calculations) by adding the concentrations of all of the dissolved species of Th, Np, and Am, respectively, in the column entitled "Molarity" in "Table of Concentrations for Batch System." Downes (2003) imported these tables into Microsoft Excel 2000 spreadsheets, and then sorted the species by radioelement and by dissolved and solid species. Finally, she added the concentrations of all of the dissolved species for each radioelement to obtain the solubilities of Th, Np, and Am (see Table 7).

We will use the same procedure to obtain Th, Np, and Am solubilities from the other runs shown in Table 2; and to obtain the compositions of Brine A, GWB, and ERDA-6 after equilibration with minerals such as halite, anhydrite, brucite, and calcite, magnesite, hydromagnesite (both $Mg_4(CO_3)_3(OH)_2 \cdot 3H_2O$ and $Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$), and nesquehonite ($MgCO_3 \cdot 3H_2O$). (This information is not required for the CRA PA.)

We used estimates of the solubilities of U(VI) from Hobart and Moore (1996) and U.S. DOE, 1996, Appendix SOTERM, SOTERM-27 - SOTERM-28) to estimate the solubility of An(VI) for the CRA PA. (These estimates will be used for U(VI) but not for other actinides in the WIPP because Np and Pu will not persist in significant quantities in the +VI oxidation state.)

Table 6. Comparison of Density, Log f_{CO_2}, Ionic Strength (I), pH, and Relative Humidity (RH) Calculated for the PAVT and the CRA PA.

Property and Brine	PAVT, All Vectors, No Organics	CRA PA, Nonmicrobial Vectors, No Organics	CRA PA, Nonmicrobial Vectors, Organics	CRA PA, Microbial Vectors, No Organics	CRA PA, Microbial Vectors, Organics
Density, Brine A	Not reported[1]	Analysis incomplete	Analysis incomplete	Analysis incomplete	Analysis incomplete
Density, GWB	Not calculated[1]	Analysis incomplete	1.23 g/cm^3	Analysis incomplete	1.23 g/cm^3
Density ERDA-6	Not reported[1]	Analysis incomplete	1.22 g/cm^3	Analysis incomplete	1.22 g/cm^3
$\text{Log} f_{CO_2}$, Brine A	-5.50[1]	Analysis incomplete	Analysis incomplete	Analysis incomplete	Analysis incomplete
$\text{Log} f_{CO_2}$, GWB	Not calculated[1]	Analysis incomplete	-5.48	Analysis incomplete	-5.50
$\text{Log} f_{CO_2}$, ERDA-6	-5.50[1]	Analysis incomplete	-6.15	Analysis incomplete	-5.50
I, Brine A	Not reported[1]	Analysis incomplete	Analysis incomplete	Analysis incomplete	Analysis incomplete
I, GWB	Not calculated[1]	Analysis incomplete	7.54 m	Analysis incomplete	7.54 m
I, ERDA-6	Not reported[1]	Analysis incomplete	6.76 m	Analysis incomplete	6.73 m

Table 6. Comparison of Density, Log f_{CO_2}, Ionic Strength (I), pH, and Relative Humidity (RH) Calculated for the PAVT and the CRA PA (cont.).

Property and Brine	PAVT, All Vectors, No Organics	CRA PA, Nonmicrobial Vectors, No Organics	CRA PA, Nonmicrobial Vectors, Organics	CRA PA, Microbial Vectors, No Organics	CRA PA, Microbial Vectors, Organics
pH, Brine A	8.69[1]	Analysis incomplete	Analysis incomplete	Analysis incomplete	Analysis incomplete
pH, GWB	Not calculated[1]	Analysis incomplete	8.69	Analysis incomplete	8.69
pH, ERDA-6	9.24[1]	Analysis incomplete	8.99	Analysis incomplete	9.02
RH, Brine A	Not reported[1]	Analysis incomplete	Analysis incomplete	Analysis incomplete	Analysis incomplete
RH, GWB	Not calculated[1]	Analysis incomplete	73.3%	Analysis incomplete	73.3%
RH, ERDA-6	Not reported[1]	Analysis incomplete	74.8%	Analysis incomplete	74.8%

1. From Trovato (1997, Attachment 2), U.S. EPA (1998a, Table 5), U.S. EPA (1998b, Subsection 4.10.4, Tables 4.10-1, 4.10-3 and 4.10-4; and Subsection 12.4, Table 12.4-1), and U.S. EPA (1998c, Subsections 5.26–5.32 and Section 6.0, Table 6.4).

Table 7. Comparison of Actinide Solubilities Calculated (An(III), An(IV), and An(V)) or Estimated (An(VI)) for the PAVT and the CRA PA.

f_{CO_2}, pH Actinide Oxidation State, and Brine	Solubility, PAVT, All Vectors, No Organics (M)	Solubility, CRA PA, Nonmicrobial Vectors, No Organics (M)	Solubility, CRA PA, Nonmicrobial Vectors, Organics (M)	Solubility, CRA PA, Microbial Vectors, No Organics (M)	Solubility, CRA PA, Microbial Vectors, Organics (M)
An(III), Brine-A	$1.2 \times 10^{-7, 1}$	Analysis incomplete	Analysis incomplete	Analysis incomplete	Analysis incomplete
An(III), GWB	Not calculated[1]	Analysis incomplete	3.07×10^{-7}	Analysis incomplete	3.07×10^{-7}
An(III), ERDA-6	$1.3 \times 10^{-8, 1}$	Analysis incomplete	1.77×10^{-7}	Analysis incomplete	1.69×10^{-7}
An(IV), Brine-A	$1.3 \times 10^{-8, 1}$	Analysis incomplete	Analysis incomplete	Analysis incomplete	Analysis incomplete
An(IV), GWB	Not calculated[1]	Analysis incomplete	1.24×10^{-8}	Analysis incomplete	1.19×10^{-8}
An(IV), ERDA-6	$4.1 \times 10^{-8, 1}$	Analysis incomplete	5.84×10^{-9}	Analysis incomplete	2.47×10^{-8}
An(V), Brine A	$2.4 \times 10^{-7, 1}$	Analysis incomplete	Analysis incomplete	Analysis incomplete	Analysis incomplete
An(V), GWB	Not calculated[1]	Analysis incomplete	9.72×10^{-7}	Analysis incomplete	1.02×10^{-6}
An(V), ERDA-6	$4.8 \times 10^{-7, 1}$	Analysis incomplete	2.13×10^{-5}	Analysis incomplete	5.08×10^{-6}

Table 7. Comparison of Actinide Solubilities Calculated (An(III), An(IV), and An(V)) or Estimated (An(VI)) for the PAVT and the CRA PA.

f_{CO_2}, pH Actinide Oxidation State, and Brine	Solubility, PAVT, All Vectors, No Organics (M)	Solubility, CRA PA, Nonmicrobial Vectors, No Organics (M)	Solubility, CRA PA, Nonmicrobial Vectors, Organics (M)	Solubility, CRA PA, Microbial Vectors, No Organics (M)	Solubility, CRA PA, Microbial Vectors, Organics (M)
An(VI), Brine-A	$8.7 \times 10^{-6, 2}$	Not required for CRA PA	Not required for CRA PA	Not required for CRA PA	Not required for CRA PA
An(VI), GWB	Not estimated[2]	$8.7 \times 10^{-6, 3}$	$8.7 \times 10^{-6, 3}$	$8.7 \times 10^{-6, 3}$	$8.7 \times 10^{-6, 3}$
An(VI), ERDA-6	$8.8 \times 10^{-6, 2}$	$8.8 \times 10^{-6, 4}$	$8.8 \times 10^{-6, 4}$	$8.8 \times 10^{-6, 4}$	$8.8 \times 10^{-6, 4}$

1. From Trovato (1997, Attachment 2), U.S. EPA (1998a, Table 5), U.S. EPA (1998b, Subsection 4.10.4, Tables 4.10-1, 4.10-3 and 4.10-4; and Subsection 12.4, Table 12.4-1), and U.S. EPA (1998c, Subsections 5.26–5.32 and Section 6.0, Table 6.4).
2. Estimated for the CCA PA by Hobart and Moore (1996). See also U.S. DOE, 1996, Appendix SOTERM, SOTERM-27 - SOTERM-28).
3. Estimate of Hobart and Moore (1996) for Brine A applied to GWB.
4. Estimate of Hobart and Moore (1996) for ERDA-6 reapplied to ERDA-6.

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