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Sandia National Laboratories
Waste Isolation Pilot Plant

Calculation of Organic-Ligand Concentrations for the WIPP CRA-2009 PABC

Work Carried Out under Task 3 of the Analysis Plan for the Calculation of Actinide Solubilities for the WIPP PABC, AP 143, Rev. 0
WIPP:1.4.1.1:PA:QA-L:548686

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TABLE OF CONTENTS

1 INTRODUCTION

This analysis report provides the current concentrations of acetate, citrate, ethylenediaminetetraacetate (EDTA ligands), and oxalate (referred to hereafter as "organic ligands") in brines that could enter the U.S. Department of Energy's (DOE's) Waste Isolation Pilot Plant (WIPP) after closure of the waste panels. These concentrations will be used to calculate actinide solubilities for the WIPP Performance Assessment Baseline Calculations (PABC), required by the U.S. Environmental Protection Agency for the second recertification of the WIPP. This analysis described in this report was carried out under Task 3 of the analysis plan (AP) for the actinide-solubility calculations for the PABC (Brush and Xiong, 2009, Subsection 4.3).

The PA calculations carried out prior to the submittal of the DOE's second Compliance Recertification Application (CRA-2009 PA) used the same actinide solubilities established for the PABC calculations conducted after the submittal of the DOE's first Compliance Recertification Application (CRA-2004 PABC). Brush and Xiong (2005a) described the conceptual models and geochemical calculations used to establish new actinide solubilities for the CRA-2004 PABC; Brush and Xiong (2005b) calculated new concentrations of organic ligands for these calculations; and Brush (2005) provided the results of these calculations.

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

Table 1. Abbreviations, Acronyms, and Initialisms.

Abbreviation, Acronym, or Initialism	Definition
acetate	CH_3COO^- or $CH_3CO_2^-$
acetic acid	CH_3COOH or CH_3CO_2H
AP	analysis plan
C	carbon
CCA	(WIPP) Compliance Certification Application
CCDF	complementary cumulative distribution function
citrate	$(CH_2COO)_2C(OH)(COO)^{3-}$ or $(CH_2CO_2)_2C(OH)(CO_2)^{3-}$
citric acid	$(CH_2COOH)_2C(OH)(COOH)$ or $(CH_2CO_2H)_2C(OH)(CO_2H)$
CRA-2004	the first (WIPP) Compliance Recertification Application
CRA-2009	the second (WIPP) Compliance Recertification Application

Table 1 continued on next page

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

Abbreviation, Acronym, or Initialism	Definition
DBR	direct brine release (a release to the surface)
DOE	(U.S.) Department of Energy
EDTA	Typically ethylenediaminetetraacetic acid, $(CH_2COOH)_2N(CH_2)_2N(CH_2COOH)_2$ or $(CH_2CO_2H)_2N(CH_2)_2N(CH_2CO_2H)_2$. In this analysis report, we refer to ethylenediaminetetraacetate $(CH_2COO)_2N(CH_2)_2N(CH_2COO)_2)^{4-}$ or $(CH_2CO_2)_2N(CH_2)_2N(CH_2CO_2)^{4-}$ as "EDTA (ligands)," because although the Am(III) and Th(IV) models include only one EDTA complex each ($AmEDTA^-$ and $ThEDTA_4(aq)$, respectively), the Np(V) model includes three ($NpO_2H_2EDTA^-$, NpO_2HEDTA^{2-}, and NpO_2EDTA^{3-})
g	gram(s)
H	hydrogen
kg	kilogram(s)
L	liter(s)
M	molar
m	meter(s) or molal
mol	moles
N	nitrogen
Na	sodium
Na-acetate	CH_3COONa or CH_3CO_2Na
NaH_2citrate	$(CH_2COOH)_2C(OH)(COONa)$ or $(CH_2CO_2H)_2C(OH)(CO_2Na)$
NaH_3EDTA	$(CH_2COOH)_2N(CH_2)_2N(CH_2COOH)(CH_2COONa)$ or $(CH_2CO_2H)_2N(CH_2)_2N(CH_2CO_2H)(CH_2CO_2Na)$
NaH-oxalate	$(COOH)(COONa)$ or $(CO_2H)(CO_2Na)$
O	oxygen
oxalate	$(COO)^{2-}$ or $C_2O_4^{2-}$
oxalic acid	$(COOH)_2$ or $H_2C_2O_4$
PA	(WIPP) performance assessment
PABC	(WIPP) Performance Assessment Baseline Calculation(s)
PAVT	(WIPP) Performance Assessment Verification Test
WIPP	(U.S. DOE) Waste Isolation Pilot Plant
wt	weight

2 MASSES OF ORGANIC LIGANDS TO BE EMPLACED IN THE WIPP

Crawford et al. (2009, Table 4-7, row labeled "Grand Total") provided the total masses of acetic acid, sodium (Na) acetate, citric acid, Na citrate, Na EDTA, oxalic acid, and Na oxalate to be emplaced in the WIPP (see also Table 2, column labeled "CRA-2009 PABC," on the next page of this analysis report). We use the formula CH_3COONa for Na acetate and abbreviate it as "Na-acetate." We assume that Na citrate is $(CH_2COOH)_2C(OH)(COONa)$ and abbreviate it as "NaH_2citrate," that Na EDTA is $(CH_2COOH)_2N(CH_2)_2N(CH_2COOH)(CH_2COONa)$ and abbreviate it as "NaH_3EDTA," and that Na oxalate is (COOH)(COONa) and abbreviate it as "NaH-oxalate." Our assumptions that the Na citrate, Na EDTA, and Na oxalate reported by Crawford et al. (2009, Table 4-7, row labeled "Grand Total") have these compositions is conservative (see Section 3 below).

Table 2 also compares these masses to those used to calculate the concentrations of organic ligands for the five previous WIPP certification- or recertification-related PA calculations.

Table 2. Comparisons of Total Masses (kg) of Organic Compounds Used to Calculate the Concentrations of Organic Ligands for WIPP Certification- or Recertification-Related PA Calculations.

Compound	CCA and PAVT[A]	CRA-2004 PA[B]	CRA-2004 PABC & CRA-2009 PA[C]	CRA-2009 PABC[D]
Acetate	2.7×10^3	None reported	None reported	None reported
Acetic acid	None reported	2.01×10^2	1.42×10^2	1.32×10^4
Na-acetate	None reported	1.21×10^4	8.51×10^3	9.70×10^3
Citrate	2.9×10^5	None reported	None reported	None reported
Citric acid	None reported	1.69×10^3	1.19×10^3	5.68×10^3
NaH_2citrate	None reported	5.66×10^2	4.00×10^2	2.55×10^3
EDTA	4.7×10^1	None reported	None reported	None reported
NaH_3EDTA	None reported	3.63×10^1	2.56×10^1	3.54×10^2
Oxalate	3.3×10^3	None reported	None reported	None reported
Oxalic acid	None reported	1.95×10^4	1.38×10^4	2.66×10^4
NaH-oxalate	None reported	4.81×10^4	3.39×10^4	6.46×10^2

A. From U.S. DOE (1996b, Table SOTERM-4, column labeled "Inventory Amount") multiplied by a scaling factor of 2.05. U.S. DOE (1996b) obtained this scaling factor from U.S. DOE (1996a, p. 3-1). U.S. DOE (1996b, Table SOTERM-4, column labeled "Inventory Amount") referred to these as "acetate," "citrate," "EDTA," and "oxalate," respectively.

B. From Brush and Xiong (2003, Table 3, column labeled "Scaled Mass (kg)").

C. From Brush and Xiong (2005b, Table 3, column labeled "Total Mass (kg)," based on Crawford (2003), Crawford and Leigh (2003), and Leigh (2003, 2005a, 2005b).

D. From Crawford et al. (2009, Table 4-7, row labeled "Grand Total").

3 CALCULATIONS OF MOLECULAR WEIGHTS OF ORGANIC LIGANDS

We used the following atomic weights to calculate the molecular weights of acetic acid, Na-acetate, citric acid, NaH_2citrate, NaH_3EDTA, oxalic acid, and NaH-oxalate: H: 1.00794 g/mol; C: 12.0107 g/mol; N: 14.00674 g/mol; O: 15.9994 g/mol; and Na: 22.989770 g/mol (Lide, 2002). Table 3 provides the formulas for these compounds.

Table 3. Formulas and Molecular Weights of Two Forms of Four Ligands That Could Be Emplaced in the WIPP.

Compound	Formula Used in This Analysis Report	Mol Wt (g)
Acetic acid	CH_3COOH	60.0520
Na-acetate	CH_3COONa	82.0338
Citric acid	$(CH_2COOH)_2C(OH)(COOH)$	192.1235
NaH_2citrate	$(CH_2COOH)_2C(OH)(COONa)$	214.1054
EDTA	$(CH_2COOH)_2N(CH_2)_2N(CH_2COOH)_2$	292.2427
NaH_3EDTA	$(CH_2COOH)_2N(CH_2)_2N(CH_2COOH)(CH_2COONa)$	314.2246
Oxalic acid	$(COOH)_2$	90.0349
NaH-oxalate	$(COOH)(COONa)$	112.0167

Acetic acid, citric acid, EDTA, and oxalic acid contain one, three, four, and two acidic hydrogen atoms, respectively, for which Na (or other alkali or alkaline-earth metals) can substitute. Crawford et al. (2009) did not specify how many of the acidic hydrogens in their reported masses of Na citrate, Na EDTA, or Na oxalate were replaced by Na. Therefore, we assumed that only one of the acidic hydrogens was replaced with Na to calculate the molecular weights of NaH_2citrate, NaH_3EDTA, and NaH-oxalate. This assumption is conservative (i.e., it results in the highest molar quantities of the ligands citrate, EDTA, and oxalate).

We calculated the molecular weights of acetic acid, Na-acetate, citric acid, NaH_2citrate, EDTA, NaH_3EDTA, oxalic acid, and NaH-oxalate as follows:

- Acetic acid: (4 × atomic mass H) + (2 × atomic mass C) + (2 × atomic mass O) = (4 × 1.00794 g/mol) + (2 × 12.0107 g/mol) + 2 × 15.9994 g/mol) = (4.0318 + 24.0214 + 31.9988) g/mol = 60.0520 g/mol.

- Na-acetate: (3 × atomic mass H) + (2 × atomic mass C) + (2 × atomic mass O) + (1 × atomic mass Na) = (3 × 1.00794 g/mol) + (2 × 12.0107 g/mol) + 2 × 15.9994 g/mol) + (1 × 22.989770 g/mol) = (3.0238 + 24.0214 + 31.9988 + 22.989770) g/mol = 82.0338 g/mol.

- Citric acid: (8 × atomic mass H) + (6 × atomic mass C) + (7 × atomic mass O) = (8 × 1.00794 g/mol) + (6 × 12.0107 g/mol) + (7 × 15.9994 g/mol) = (8.0635 + 72.0642 + 111.9958) g/mol = 192.1235 g/mol.

- NaH_2citrate: (7 × atomic mass H) + (6 × atomic mass C) + (7 × atomic mass O) + (1 × atomic mass Na) = (7 × 1.00794 g/mol) + (6 × 12.0107 g/mol) + (7 × 15.9994 g/mol) + (1 × 22.989770 g/mol) = (7.0556 + 72.0642 + 111.9958 + 22.989770) g/mol = 214.1054 g/mol.

- EDTA: (16 × atomic mass H) + (10 × atomic mass C) + (2 × atomic mass of N) + (8 × atomic mass O) = (16 × 1.00794 g/mol) + (10 × 12.0107 g/mol) + (2 × 14.00674 g/mol) + (8 × 15.9994 g/mol) = (16.1270 + 120.1070 + 28.0135 + 127.9952) g/mol = 292.2427 g/mol.

- NaH_3EDTA: (15 × atomic mass H) + (10 × atomic mass C) + (2 × of N) + (8 × atomic mass O) + (1 × atomic mass Na)= (15 × 1.00794 g/mol) + (10 × 12.0107 g/mol) + (2 × 14.00674 g/mol) + (8 × 15.9994 g/mol) + (1 × 22.989770 g/mol) = (15.1191 + 120.1070 + 28.0135 + 127.9952 + 22.989770) g/mol = 314.2246 g/mol.

- Oxalic acid: (2 × atomic mass H) + (2 × atomic mass C) + (4 × atomic mass O) = (2 × 1.00794 g/mol) + (2 × 12.0107 g/mol) + 4 × 15.9994 g/mol) = (2.0159 + 24.0214 + 63.9976) g/mol = 90.0349 g/mol.

- NaH-oxalate: (1 × atomic mass H) + (2 × atomic mass C) + (4 × atomic mass O) + (1 × atomic mass Na) = (1 × 1.00794 g/mol) + (2 × 12.0107 g/mol) + 4 × 15.9994 g/mol) + (1 × 22.989770 g/mol) = (1.00794 + 24.0214 + 63.9976 + 22.989770) g/mol = 112.0167 g/mol.

Table 3 lists the molecular weights of these compounds (see preceding page).

4 BRINE VOLUME USED TO CALCULATE ORGANIC-LIGAND CONCENTRATIONS

We used 17,400 m^3 of brine, "[A] reasonable minimum volume of brine in the repository required for a DBR [direct brine release]" (Clayton, 2008), to calculate the dissolved concentrations of acetate, citrate, EDTA (ligands), and oxalate in a homogeneous, 10-panel PA repository. A volume of 17,400 m^3 of brine is conservative because any volume greater than 17,400 m^3 would result in lower organic-ligand concentrations. A volume of 17,400 m^3 of brine is equal to 17,400,000 L of brine.

Table 4 (see next page) compares the brine volumes used to calculate the concentrations of organic ligands for all six WIPP certification- or recertification-related PA calculations. Table 4 shows that the minimum brine volume increased by a factor of 1.74 since the CRA-2004 PABC and the CRA-2009 PA.

The previous estimates of the minimum volume of brine in the repository required for a DBR were based on the results of the PA calculations carried out prior to those in which the dissolved concentrations of organic ligands calculated using these estimates were used to establish new actinide solubilities. For example, Stein (2005) used the results of the CRA-2004 PA calculations to estimate a new minimum brine volume of 10,011 m^3, which was used for the actinide-solubility calculations for the CRA-2004 PABC and the CRA-2009 PA. Clayton's main objective for estimating a new minimum brine volume for the CRA-2009 PABC was to establish a method that is independent of the results of any given PA calculation. Therefore, it is expected that this estimate will not change in the future. Clayton (2008) provided a detailed description of how the new minimum brine volume was estimated.

Table 4. Comparisons of Brine Volumes (m^3) Used to Calculate the Concentrations of Organic Ligands for WIPP Certification- or Recertification-Related PA Calculations.

	CCA, PAVT & CRA-2004 PA[A]	CRA-2004 PABC & CRA-2009 PA[B]	CRA-2009 PABC[C]
Minimum Brine Volume (m^3)	29,841	10,011	17,400

A. [T]he smallest quantity of brine required to be in the repository [for] transport away from the repository" (Larson, 1996)
B. "[A] reasonable minimum volume of brine in the repository required for a brine release" (Stein, 2005).
C. "[A] reasonable minimum volume of brine in the repository required for a DBR" (Clayton, 2008).

5 CALCULATION OF ORGANIC-LIGAND CONCENTRATIONS

We calculated the concentrations of acetic acid, Na-acetate, citric acid, NaH_2citrate, NaH_3EDTA, oxalic acid, and NaH-oxalate by multiplying the total masses of these compounds in kg from Table 2 of this report, column labeled "CRA-2009 PABC," by 1000 g/kg to convert these estimates of the total masses in kg (Crawford et al., 2009) to grams. Next, we divided these masses by the molecular weights of these compounds from Table 3 of this report, column labeled "Mol Wt (g)," which yielded the total quantities of these compounds to be emplaced in moles. We then divided these quantities by 17,400,000 L to obtain the concentrations of these compounds in units of mol/L, or M:

- Acetic acid: $((1.32 \times 10^4 \text{ kg}) \times (1000 \text{ g/kg}) \div (60.0520 \text{ g/mol})) \div 1.74 \times 10^7 \text{ L} = 1.26 \times 10^{-2}$ M.
- Na-acetate: $((9.70 \times 10^3 \text{ kg}) \times (1000 \text{ g/kg}) \div (82.0338 \text{ g/mol})) \div 1.74 \times 10^7 \text{ L} = 6.80 \times 10^{-3}$ M.
- Citric acid: $((5.68 \times 10^3 \text{ kg}) \times (1000 \text{ g/kg}) \div (192.1235 \text{ g/mol})) \div 1.74 \times 10^7 \text{ L} = 1.70 \times 10^{-3}$ M.
- NaH_2citrate: $((2.55 \times 10^3 \text{ kg}) \times (1000 \text{ g/kg}) \div (214.1054 \text{ g/mol})) \div 1.74 \times 10^7 \text{ L} = 6.84 \times 10^{-4}$ M.

- NaH_3EDTA: $((3.54 \times 10^2 \text{ kg}) \times (1000 \text{ g/kg}) \div (314.2246 \text{ g/mol})) \div 1.74 \times 10^7 \text{ L} = 6.47 \times 10^{-5}$ M.

- Oxalic acid: $((2.66 \times 10^4 \text{ kg}) \times (1000 \text{ g/kg}) \div (90.0349 \text{ g/mol})) \div 1.74 \times 10^7 \text{ L} = 1.70 \times 10^{-2}$ M.

- NaH-oxalate: $((6.46 \times 10^2 \text{ kg}) \times (1000 \text{ g/kg}) \div (112.0167 \text{ g/mol})) \div 1.74 \times 10^7 \text{ L} = 3.31 \times 10^{-4}$ M.

We calculated the total dissolved concentrations of acetate, citrate, and oxalate by adding the concentrations of acetic acid and Na-acetate; citric acid and NaH_2citrate; and oxalic acid and NaH-oxalate. The total concentration of EDTA (ligands) is equal to the concentration of NaH_3EDTA.

Table 5 summarizes our calculations in this report.

Table 5. Summary of Our Calculations of the Dissolved Concentrations of One or Two Forms of Four Organic Ligands and the Total Concentrations of These Ligands for a Homogeneous, 10-Panel Repository.

Compound	Total Mass (kg)[A]	Total Mass (g)	Total Quantity (mol)[B]	Concentration (M)[C]
Acetic acid	1.32×10^{4}	1.32×10^{7}	2.20×10^{5}	1.26×10^{-2}
Na-acetate	9.70×10^{3}	9.70×10^{6}	1.18×10^{5}	6.80×10^{-3}
Total acetate	-	-	-	1.94×10^{-2}
Citric acid	5.68×10^{3}	5.68×10^{6}	2.96×10^{4}	1.70×10^{-3}
NaH_2citrate	2.55×10^{3}	2.55×10^{6}	1.19×10^{4}	6.84×10^{-4}
Total citrate	-	-	-	2.38×10^{-3}
EDTA	None reported	None reported	None reported	None reported
NaH_3EDTA	3.54×10^{2}	3.54×10^{5}	1.13×10^{3}	6.47×10^{-5}
Total EDTA (ligands)	-	-	-	6.47×10^{-5}
Oxalic acid	2.66×10^{4}	2.66×10^{7}	2.95×10^{5}	1.70×10^{-2}
NaH-oxalate	6.46×10^{2}	6.46×10^{5}	5.77×10^{3}	3.31×10^{-4}
Total oxalate	-	-	-	1.73×10^{-2}

A. From Crawford et al. (2009, Table 4-7, row labeled "Grand Total") and Table 2 of this report, column labeled "CRA-2009 PABC."
B. Based on Lide (2002) and results in Table 3, column labeled "Mol Wt (g)."
C. Based on a minimum brine volume of 17,400 m^3 or 17,400,000 L (Clayton (2008).

6 COMPARISONS WITH PREVIOIUS RESULTS

Table 6 compares our new total dissolved concentrations of acetate, citrate, EDTA (ligands), and oxalate for a homogeneous, 10-panel repository and to the concentrations used to calculate actinide speciation and solubilities for WIPP certification- or recertification-related PA calculations. Table 6 shows that the dissolved concentration of acetate increased by a factor of 1.83; the concentration of citrate increased by a factor of 2.95; the concentration of EDTA increased by a factor of 7.95; and the concentration of oxalate decreased by a factor of 2.63 since the CRA-2004 PABC and the CRA-2009 PA.

The results of Brush et al. (2008, Figures 1 and 2) can be used to estimate the effects of an eight-fold increase in the EDTA (ligands) concentration on the mean complementary cumulative distribution function (CCDF) for direct brine releases (DBRs) and the mean CCDF for total releases from the repository. We cannot estimate the effects of the increases in the concentrations of acetate or citrate or the decrease in the concentration of oxalate, but we expect that the actinide speciation and solubility calculations for the CRA-2009 PABC will show that these changes will have less effect on actinide solubilities than the change in the EDTA (ligands) concentration.

Table 6. Comparisons of Organic-Ligand Concentrations Used to Calculate Actinide Speciation and Solubilities for WIPP Certification- or Recertification-Related PA Calculations.

Organic Ligand	CCA[A] and PAVT (m)	CRA-2004 PA[B] (M)	CRA-2004 PABC[C] and CRA-2009 PA (M)	CRA-2009 PABC[D] (M)
Total Acetate	1.1×10^{-3}	5.05×10^{-3}	1.06×10^{-2}	1.94×10^{-2}
Total Citrate	7.4×10^{-3}	3.83×10^{-4}	8.06×10^{-4}	2.38×10^{-3}
Total EDTA (ligands)	4.2×10^{-6}	3.87×10^{-6}	8.14×10^{-6}	6.47×10^{-5}
Total Oxalate	4.7×10^{-4}	2.16×10^{-2}	4.55×10^{-2}	1.73×10^{-2}

A. U.S. DOE (1996b, Appendix SOTERM, Table SOTERM-4, column labeled "Organic Concentration (scaled)."
B. Brush and Xiong (2003, Table 4, column labeled "CRA Concentration (M)").
C. Brush and Xiong (2005b, Table 4, column labeled "PABC (M)").
D. This report.

7 CONCLUSIONS

This analysis yielded the following organic-ligand concentrations for the actinide speciation and solubility calculations for the CRA-2009 PABC: (1) acetate: 1.94×10^{-2} M, (2) citrate: 2.38×10^{-3} M; (3) EDTA (ligands): 6.47×10^{-5} M; and (4) oxalate: 1.73×10^{-2} M (see Table 5 or 6 above).

The dissolved concentration of acetate increased by a factor of 1.83; the concentration of citrate increased by a factor of 2.95; the concentration of EDTA increased by a factor of 7.95; and the concentration of oxalate decreased by a factor of 2.63 since the CRA-2004 PABC and the CRA-2009 PA (Table 6).

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