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Sandia National Laboratories
Waste Isolation Pilot Plant

Calculation of Organic-Ligand Concentrations for the WIPP CRA-2014 PA

Work Carried Out under Task 5 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 new concentrations of the organic ligands acetate, citrate, ethylenediaminetetraacetate (EDTA), and oxalate dissolved in two standard Waste Isolation Pilot Plant (WIPP) brines as a function of the volumes of these brines in the repository. These brines 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.

We will use these concentrations to predict the baseline actinide solubilities in the performance assessment (PA) calculations 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 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., 2012, 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
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 $(CH_2CO_2)_2C(OH)(CO_2)^{3-}$

Table 1 continued on next page.

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

Abbreviation, Acronym, or Initialism	Definition
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
DBR	direct brine release (a release to the surface)
CRA-2009	the second (WIPP) Compliance Recertification Application
DOE	(U.S.) Department of Energy
EDTA	ethylenediaminetetraacetic acid, $(CH_2COOH)_2N(CH_2)_2N(CH_2COOH)_2$ or $(CH_2CO_2H)_2N(CH_2)_2N(CH_2CO_2H)_2$.
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	Waste Isolation Pilot Plant
wt	weight

2 MASSES OF ORGANIC LIGANDS TO BE EMPLACED IN THE WIPP

Van Soest (2012, Table 5-9) provided the total masses of acetate, acetic acid, citrate, citric acid, EDTA, oxalate, and oxalic acid to be emplaced in the WIPP. Table 2, column labeled "CRA-2014 PA," of this analysis report (see next page) contains these masses from Van Soest (2012).

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. Acetate, citrate, ethylenediaminetetraacetate, and oxalate are the deprotonated forms of these acids, and have charges of –1, –3, –4, and –2, respectively; these deprotonated species are referred to as "ligands." Table 1 (see Section 1 above) provides the formulas for these acids and ligands. Acetate, citrate, ethylenediaminetetraacetate, and oxalate cannot exist by themselves in TRU waste, because they are charged species. Instead, they must be accompanied by positively charged species such as protons (H^+) or Na^+. For this analysis, it was assumed that the acetate, citrate, and oxalate reported by Van Soest (2012) are actually present as acetic acid, citric acid, and oxalic acid, respectively; and that the EDTA reported by Van Soest (2012) is fully protonated (i.e., that the EDTA is present in the waste as ethylenediaminetetraacetic acid, not ethylenediaminetetraacetate). This is conservative, because assuming the presence of any positively charged species with an atomic mass greater than that of H^+ (e.g., Na^+) would decrease the number of moles of ligands present in the waste and brine.

Table 2 also compares the masses of acetate, acetic acid, citrate, citric acid, EDTA, oxalate, and oxalic acid reported by Van Soest (2012) to those used to calculate the concentrations of organic ligands for the five previous WIPP certification- or recertification-related PA calculations. Note that masses of acetic acid, Na acetate, citric acid, Na citrate, Na EDTA, oxalic acid, and Na oxalate were reported for the CRA-2004 PA, the CRA-2004 PABC and CRA 2009 PA, and the CRA-2009 PABC, instead of acetate, acetic acid, citrate, citric acid, EDTA, oxalate, and oxalic acid. Reporting the masses of acetate, acetic acid, citrate, citric acid, EDTA, oxalate, and oxalic acid was conservative, because reporting the presence of Na-containing forms of these compounds would decrease the number of moles of these ligands present in the waste and brine.

Note also that the inventory reports used for the CRA-2004 PA, the CRA-2004 PABC and CRA 2009 PA, and the CRA-2009 PABC did not specify how many of the acidic hydrogen atoms in their reported masses of Na citrate, Na EDTA, or Na oxalate were replaced by Na. Therefore, Brush and Xiong (2003; 2005; 2009) assumed that only one of the acidic hydrogen atoms was replaced with Na to calculate the molecular weights of NaH_2citrate, NaH_3EDTA, and NaH-oxalate. This assumption was also conservative (i.e., it resulted in the highest molar quantities of the ligands citrate, EDTA, and oxalate).

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]	CRA-2014 PA[E]
Acetate	2.7×10^3	None reported	None reported	None reported	9.96×10^3
Acetic acid	None reported	2.01×10^2	1.42×10^2	1.32×10^4	1.41×10^4
Na-acetate	None reported	1.21×10^4	8.51×10^3	9.70×10^3	None reported
Citrate	2.9×10^5	None reported	None reported	None reported	2.55×10^3
Citric acid	None reported	1.69×10^3	1.19×10^3	5.68×10^3	5.23×10^3
NaH_2citrate	None reported	5.66×10^2	4.00×10^2	2.55×10^3	None reported
EDTA	4.7×10^1	None reported	None reported	None reported	3.76×10^2
NaH_3EDTA	None reported	3.63×10^1	2.56×10^1	3.54×10^2	None reported
Oxalate	3.3×10^3	None reported	None reported	None reported	6.50×10^2
Oxalic acid	None reported	1.95×10^4	1.38×10^4	2.66×10^4	1.78×10^4
NaH-oxalate	None reported	4.81×10^4	3.39×10^4	6.46×10^2	None reported

Footnotes for Table 2 provided on next page.

Footnotes for Table 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 Crawford (2003); used by Brush and Xiong (2003).
C. From Crawford (2003), Crawford and Leigh (2003), and Leigh (2003, 2005a, 2005b); used by Brush and Xiong (2005).
D. From Crawford et al. (2009); used by Brush and Xiong (2009).
E. From Van Soest (2012); used for this analysis report.

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3 CALCULATIONS OF MOLECULAR WEIGHTS OF ORGANIC LIGANDS

We used the following atomic weights to calculate the molecular weights of acetic acid, citric acid, EDTA, and oxalic acid: 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).

We calculated the molecular weights of acetic acid, citric acid, EDTA, and oxalic acid 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.

- 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.

- 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.

- 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.

Table 3 summarizes the molecular weights of 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
Citric acid	$(CH_2COOH)_2C(OH)(COOH)$	192.1235
EDTA	$(CH_2COOH)_2N(CH_2)_2N(CH_2COOH)_2$	292.2427
Oxalic acid	$(COOH)_2$	90.0349

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4 BRINE VOLUME USED TO CALCULATE ORGANIC-LIGAND CONCENTRATIONS

We used five different volumes of GWB or ERDA-6 to calculate the concentrations of acetate, citrate, EDTA, and oxalate for the CRA-2014 PA. First, 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 maximum dissolved concentrations of these organic ligands in a homogeneous, 10-panel PA repository. A DBR is defined as a release of brine that occurs 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.). We calculated these maximum concentrations by assuming that the total masses of these ligands in the waste would dissolve completely in this volume of brine.

We then recalculated the concentrations of acetate, citrate, EDTA, and oxalate for brine volumes that are 2, 3, 4, or 5 times this minimum volume by dividing these maximum concentrations by 2, 3, 4, or 5, respectively. We used factors of 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 the minimum brine volume and 5 times the minimum volume.

Table 4 (see next page) compares the brine volumes used to calculate the concentrations of organic ligands for all seven WIPP certification- or recertification-related PA calculations. The previous estimates of the minimum volume of brine in the repository required for a DBR were based on the results of previous PA calculations. 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 (2008), however, successfully established a minimum brine volume 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 this minimum volume was established.

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

Brine Volume	CCA, PAVT & CRA-2004 PA[A]	CRA-2004 PABC & CRA-2009 PA[B]	CRA-2009 PABC[C]	CRA-2014 PA[C, D]
Minimum	29,841	10,011	17,400	17,400
Additional volume for CRA-2014 PA	-	-	-	34,800 (2 × min.)
Additional volume for CRA-2014 PA	-	-	-	52,200 (3 × min)
Additional volume for CRA-2014 PA	-	-	-	69,600 (4 × min)
Additional volume for CRA-2014 PA	-	-	-	87,000 (5 × min)

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).
D. Also used 2 ×, 3 ×, 4 ×, and 5 × the minimum brine volume of Clayton (2008).

5 CALCULATION OF ORGANIC-LIGAND CONCENTRATIONS

We calculated the concentrations of acetic acid, citric acid, EDTA, and oxalic acid by adding the masses of acetate and acetic acid, citrate and citric acid, and oxalate and oxalic acid from Table 2 of this report (column labeled "CRA-2014 PA"). This is because we assumed that acetate, citrate, and oxalate are actually present in TRU waste as acetic acid, citric acid, and oxalic acid (see Section 2 above). We then multiplied the total masses of these compounds and EDTA in kg by 1000 g/kg to convert them from kg to grams. Next, we divided these masses by the molecular weights of these compounds from Table 3 of this report, which yielded the total quantities of these compounds to be emplaced in moles. Finally, we divided these molar quantities by 17,400,000 L, because a volume of 17,400 m^3 of brine is equal to 17,400,000 L, to obtain the concentrations of these compounds in units of mol/L, or M:

- Acetic acid: $((9.96 \times 10^3 \text{ kg} + 1.41 \times 10^4 \text{ kg}) \times (1000 \text{ g/kg}) \div (60.0520 \text{ g/mol})) \div 1.74 \times 10^7 \text{ L} = 2.30 \times 10^{-2}$ M.

- Citric acid: $((2.55 \times 10^3 \text{ kg} + 5.23 \times 10^3 \text{ kg}) \times (1000 \text{ g/kg}) \div (192.1235 \text{ g/mol})) \div 1.74 \times 10^7 \text{ L} = 2.33 \times 10^{-3}$ M.

- EDTA: $((3.76 \times 10^2 \text{ kg}) \times (1000 \text{ g/kg}) \div (292.2427 \text{ g/mol})) \div 1.74 \times 10^7 \text{ L} = 7.40 \times 10^{-5}$ M.

- Oxalic acid: $((6.50 \times 10^2 \text{ kg} + 1.78 \times 10^4 \text{ kg}) \times (1000 \text{ g/kg}) \div (90.0349 \text{ g/mol})) \div 1.74 \times 10^7 \text{ L} = 1.18 \times 10^{-2}$ M.

Table 5 (see next page) summarizes our calculations the dissolved concentrations of these organic ligands in the minimum volume of brine required for a DBR from a homogeneous, 10-Panel Repository. The intermediate results have been rounded to three significant figures for entry in Table 5. However, we did not round off until we obtained the final concentrations in our calculations.

Table 6 (next page) provides the dissolved concentrations of acetate, citrate, EDTA, and oxalate for the minimum brine volume of 17,400 m^3 and for volumes that are 2, 3, 4, or 5 times this minimum volume. In this table, we report our final reposts as ligands, not acids, because the ligands would potentially form complexes with the actinide elements in the TRU waste that is being emplaced in the WIPP. The intermediate results have been rounded to three significant figures for entry in Table 6. However, we did not round off until we obtained the final concentrations in our calculations.

We first calculated all of the results shown in Tables 5 and 6 with a hand calculator, then checked them with an Excel spreadsheet (AP-153, Rev 1_Task 5_Org Lig Concs.xlsx). We will place this spreadsheet in the SNL/WIPP Records Center along with all other records for AP-153, Task 5.

Table 5. Summary of Our Calculations of the Dissolved Concentrations of Organic Ligands in the Minimum Volume of Brine Required for a DBR from a Homogeneous, 10-Panel Repository.

Compound	Total Mass (kg)	Total Mass (g)	Total Quantity (mol)	Concentration (M)
Acetic acid	2.41×10^{4}	2.41×10^{7}	4.01×10^{5}	2.30×10^{-2}
Citric acid	7.78×10^{3}	7.78×10^{6}	4.05×10^{4}	2.33×10^{-3}
EDTA	3.76×10^{2}	3.76×10^{5}	1.29×10^{3}	7.40×10^{-5}
Oxalic acid	1.84×10^{4}	1.84×10^{7}	2.05×10^{5}	1.18×10^{-2}

Table 6. 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}

6 COMPARISONS WITH PREVIOIUS RESULTS

Table 6 (see Section 5 above) provides the concentrations of acetate, citrate, EDTA, and oxalate that will be used for the baseline actinide-solubility calculations for the CRA-2014 PA. Table 6 provides these concentrations for the minimum volume of GWB or ERDA-6 (17,400 m^3) required for a DBR from the repository, and for volumes that are 2, 3, 4, or 5 times this minimum volume. Table 7 (see below) compares our new acetate, citrate, EDTA, and oxalate concentrations calculated for the minimum brine volume to those used for previous certification- or recertification-related PA calculations. Inspection of Tables 6 and 7 shows that the concentrations of acetate and EDTA in the minimum brine volume increased somewhat from those calculated for the CRA-2009 PABC, but that the concentrations of citrate and oxalate decreased. However, Tables 6 and 7 also show that all of the organic-ligand concentrations calculated for brine volumes that are 2, 3, 4, or 5 times the minimum volume are less than those used previously.

We do not anticipate these changes will affect the results of the CRA-2014 PA significantly.

Table 7. Comparison of the Dissolved Concentrations of Organic Ligands in the Minimum Volume of Brine Required for a DBR from a Homogeneous, 10-Panel Repository.

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)	CRA-2014 PA[E] (M)
Acetate	1.1×10^{-3}	5.05×10^{-3}	1.06×10^{-2}	1.94×10^{-2}	2.30×10^{-2}
Citrate	7.4×10^{-3}	3.83×10^{-4}	8.06×10^{-4}	2.38×10^{-3}	2.33×10^{-3}
EDTA	4.2×10^{-6}	3.87×10^{-6}	8.14×10^{-6}	6.47×10^{-5}	7.40×10^{-5}
Oxalate	4.7×10^{-4}	2.16×10^{-2}	4.55×10^{-2}	1.73×10^{-2}	1.18×10^{-2}

A. U.S. DOE (1996b, Appendix SOTERM, Table SOTERM-4)
B. Brush and Xiong (2003)
C. Brush and Xiong (2005)
D. Brush and Xiong (2009)
E. This report

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7 CONCLUSIONS

This analysis report provides updated concentrations of the organic ligands acetate, citrate, EDTA, and oxalate dissolved in GWB and ERDA-6 as a function of the volume of these brines in the repository. These concentrations will be used to calculate the baseline actinide solubilities as a function of brine volume for the CRA-2014 PA. This PA will use solubilities that depend on the volume of brine released from the repository.

Table 6 (see Section 5 above) provides the concentrations of acetate, citrate, EDTA, and oxalate that will be used for the baseline actinide-solubility calculations for the CRA-2014 PA. Table 6 provides these concentrations for the minimum volume of GWB or ERDA-6 (17,400 m^3) required for a DBR from the repository, and for volumes that are 2, 3, 4, or 5 times this minimum volume. Table 7 (Section 6) compares our new acetate, citrate, EDTA, and oxalate concentrations calculated for the minimum brine volume to those used for previous certification- or recertification-related PA calculations. Inspection of Tables 6 and 7 shows that the concentrations of acetate and EDTA in the minimum brine volume increased somewhat from those calculated for the CRA-2009 PABC, but that the concentrations of citrate and oxalate decreased. However, Tables 6 and 7 also show that all of the organic-ligand concentrations calculated for brine volumes that are 2, 3, 4, or 5 times the minimum volume are less than those used previously.

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