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Sandia National Laboratories
Waste Isolation Pilot Plant

Calculation of Organic-Ligand Concentrations for the WIPP CRA-2019 Deferred PA

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

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1 INTRODUCTION

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 fourth recertification of the WIPP by the U.S. Environmental Protection Agency (EPA) (the 2019 Compliance Recertification Application, or CRA-2019 Deferred 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).

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
CRA-2014	the third (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 (2018, 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-2019 PA," of this analysis report (see next page) contains these masses from Van Soest (2018).

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 ions. 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 ions 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 (2018) 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. In CRA-2014 and CRA-2019 this changed and instead what was reported was 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 ions 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 ions 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 higher molar quantities of the ligands citrate, EDTA, and oxalate rather than using their salt forms with a higher number of Na^+).

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	CRA-2004 PA[B]	CRA-2004 PABC & CRA-2009 PA[C]	CRA-2009 PABC[D]	CRA-2014 PA[E]	CRA-2019 PA[F]
Acetate	None reported	None reported	None reported	9.96×10^3	**1.37×10^4**
Acetic acid	2.01×10^2	1.42×10^2	1.32×10^4	1.41×10^4	**1.59×10^4**
Na-acetate	1.21×10^4	8.51×10^3	9.70×10^3	None reported	None reported
Citrate	None reported	None reported	None reported	2.55×10^3	**2.63×10^3**
Citric acid	1.69×10^3	1.19×10^3	5.68×10^3	5.23×10^3	**5.08×10^3**
NaH_2citrate	5.66×10^2	4.00×10^2	2.55×10^3	None reported	None reported
EDTA	None reported	None reported	None reported	3.76×10^2	**4.03×10^2**
NaH_3EDTA	3.63×10^1	2.56×10^1	3.54×10^2	None reported	None reported
Oxalate	None reported	None reported	None reported	6.50×10^2	**7.00×10^2**
Oxalic acid	1.95×10^4	1.38×10^4	2.66×10^4	1.78×10^4	**1.70×10^4**
NaH-oxalate	4.81×10^4	3.39×10^4	6.46×10^2	None reported	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)
F. From Van Soest (2018); used for this analysis report.

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

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-2019 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. This method is consistent with the approach used in the CRA-2014 PA.

Table 4 (see next page) compares the brine volumes used to calculate the concentrations of organic ligands for all eight 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 & CRA-2019[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 CALCULATIONS 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: $((1.37 \times 10^4 \text{ kg} + 1.59 \times 10^4 \text{ kg}) \times (1000 \text{ g/kg}) \div (60.0520 \text{ g/mol})) \div 1.74 \times 10^7 \text{ L} = 2.83 \times 10^{-2}$ M.

- Citric acid: $((2.63 \times 10^3 \text{ kg} + 5.08 \times 10^3 \text{ kg}) \times (1000 \text{ g/kg}) \div (192.1235 \text{ g/mol})) \div 1.74 \times 10^7 \text{ L} = 2.30 \times 10^{-3}$ M.

- EDTA: $((4.03 \times 10^2 \text{ kg}) \times (1000 \text{ g/kg}) \div (292.2427 \text{ g/mol})) \div 1.74 \times 10^7 \text{ L} = 7.92 \times 10^{-5}$ M.

- Oxalic acid: $((7.00 \times 10^2 \text{ kg} + 1.70 \times 10^4 \text{ kg}) \times (1000 \text{ g/kg}) \div (90.0349 \text{ g/mol})) \div 1.74 \times 10^7 \text{ L} = 1.13 \times 10^{-2}$ 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_CRA2019.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 (17,400 m^3) Required for a DBR from a Homogeneous, 10-Panel Repository.

Compound	Total Mass (kg)	Total Mass (g)	Total Quantity (mol)	Concentration (M)
Acetic acid	2.96×10^4	2.96×10^7	4.93×10^5	2.83×10^{-2}
Citric acid	7.70×10^3	7.70×10^6	4.01×10^4	2.30×10^{-3}
EDTA	4.03×10^2	4.03×10^5	1.39×10^3	7.92×10^{-5}
Oxalic acid	1.77×10^4	1.77×10^7	1.97×10^5	1.13×10^{-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	2.83×10^{-2}	1.42×10^{-2}	9.45×10^{-3}	7.09×10^{-3}	5.67×10^{-3}
Citrate	2.30×10^{-3}	1.15×10^{-3}	7.68×10^{-4}	5.76×10^{-4}	4.61×10^{-4}
EDTA	7.92×10^{-5}	3.96×10^{-5}	2.64×10^{-5}	1.98×10^{-5}	1.58×10^{-5}
Oxalate	1.13×10^{-2}	5.65×10^{-3}	3.77×10^{-3}	2.82×10^{-3}	2.26×10^{-3}

6 COMPARISONS WITH PREVIOUS 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-2019 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 trend concentrations for the organic ligands in the minimum brine volume remained consistent with that seen for CRA-2014 (acetate and EDTA increased, whereas the concentrations for citrate and oxalate decreased).

We do not anticipate these changes will affect the results of the CRA-2019 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	CRA-2004 PA[B] (M)	CRA-2004 PABC[C] and CRA-2009 PA (M)	CRA-2009 PABC[D] (M)	CRA-2014 PA[E] (M)	CRA-2019 PA[F] (M)
Acetate	5.05×10^{-3}	1.06×10^{-2}	1.94×10^{-2}	2.30×10^{-2}	2.83×10^{-2}
Citrate	3.83×10^{-4}	8.06×10^{-4}	2.38×10^{-3}	2.33×10^{-3}	2.30×10^{-3}
EDTA	3.87×10^{-6}	8.14×10^{-6}	6.47×10^{-5}	7.40×10^{-5}	7.92×10^{-5}
Oxalate	2.16×10^{-2}	4.55×10^{-2}	1.73×10^{-2}	1.18×10^{-2}	1.13×10^{-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. Brush and Domski (2013)
F. This Report

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-2019 Deferred 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-2019 Deferred 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-2014, but that the concentrations of citrate and oxalate decreased.

8 REFERENCES

Brush, L.H., P.S. Domski, and Y.-L. Xiong. 2012. "Analysis Plan for WIPP Near-Field Geochemical Process Modeling." AP-153, Rev. 1, February 8, 2012. Carlsbad, NM: Sandia National Laboratories. ERMS 556960.

Brush, L.H., P.S. Domski 2013. "Calculation of Organic-Ligand Concentrations for the WIPP CRA-2014 PA" Analysis Report, January 14, 2013. Carlsbad, NM: Sandia National Laboratories. ERMS 559005.

Brush, L.H., and Y.-L. Xiong. 2003. "Calculation of Organic Ligand Concentrations for the WIPP Compliance Recertification Application." Analysis report, April 14, 2003. Carlsbad, NM: Sandia National Laboratories. ERMS 527567.

Brush, L.H., and Y.-L. Xiong. 2005. "Calculation of Organic-Ligand Concentrations for the WIPP Performance-Assessment Baseline Calculations." Analysis report, May 4, 2005. Carlsbad, NM: Sandia National Laboratories. ERMS 539635.

Brush, L.H., and Y.-L. Xiong, 2009. "Calculation of Organic-Ligand Concentrations for the WIPP CRA-2009 PABC." Analysis Report, June 16, 2009. Carlsbad, NM: Sandia National Laboratories. ERMS 551481.

Clayton, D.J. 2008. "Update to the Calculation of the Minimum Brine Volume for a Direct Brine Release." Memorandum to L.H. Brush, April 2, 2008. Carlsbad, NM: Sandia National Laboratories. ERMS 548522.

Crawford, B.A. 2003. "Updated Estimate of Complexing Agents in Transuranic Solidified Waste Forms Scheduled for Disposal and Emplaced at WIPP." Letter to C.D. Leigh, April 8, 2003. Carlsbad, NM: Los Alamos National Laboratory. ERMS 527409.

Crawford, B.A., D. Guerin, S. Lott, B. McInroy, J. McTaggart, and G. Van Soest. 2009. "Performance Assessment Inventory Report – 2008." INV-PA-08, Rev 0. Carlsbad, NM: Los Alamos National laboratory – Carlsbad Operations.

Crawford, B.A., and C.D. Leigh. 2003. "Estimate of Complexing Agents in TRU Waste for the Compliance Recertification Application." Analysis report, August 28, 2003. Carlsbad, NM: Los Alamos National Laboratory. ERMS 531107.

Krumhansl, J.L., K.M. Kimball, and C.L. Stein. 1991. *Intergranular Fluid Compositions from the Waste Isolation Pilot Plant (WIPP), Southeastern New Mexico*. SAND90-0584. Albuquerque, NM: Sandia National Laboratories.

Larson, K.W. 1996. "Brine-Waste Contact Volumes for Scoping Analysis of Organic Ligand Concentration." Memorandum to R.V. Bynum, March 13, 1996. Albuquerque, NM: Sandia National Laboratories. ERMS 236044.

Leigh, C.D. 2003. "New Estimates of the Total Masses of Complexing Agents in the WIPP Inventory for Use in the 2003 WIPP Performance Assessment." Memorandum to L.H. Brush, September 3, 2003. Carlsbad, NM: Sandia National Laboratories. ERMS 531319.

Leigh, C.D. 2005a. "Organic Ligand Masses TRU Waste Streams from TWBID Revision 2.1 Version 3.13 Data Version D4.15." Memorandum to L.H. Brush, April 14, 2005, Carlsbad, NM: Sandia National Laboratories. ERMS 539354.

Leigh, C.D. 2005b. "Organic Ligand Masses TRU Waste Streams from TWBID Revision 2.1, Version 3.13, Data Version D4.15, Revisions 1." Memorandum to L.H. Brush, April 18, 2005, Carlsbad, NM: Sandia National Laboratories. ERMS 539550.

Lide, D.R. 2002. *CRC Handbook of Chemistry and Physics*, 83rd edition. Boca Raton, FL: CRC Press.

Popielak, R.S., R.L. Beauheim, S.R. Black, W.E. Coons, C.T. Ellingson and R.L. Olsen. 1983. *Brine Reservoirs in the Castile Formation, Waste Isolation Pilot Plant Project, Southeastern New Mexico*. TME 3153. Carlsbad, NM: U.S. Department of Energy WIPP Project Office.

Snider, A.C. 2003. "Verification of the Definition of Generic Weep Brine and the Development of a Recipe for This Brine." Analysis report, April 8, 2003. Carlsbad, NM: Sandia National Laboratories. ERMS 527505.

Stein, J.S. 2005. "Estimate of Volume of Brine in Repository That Leads to a Brine Release." Memorandum to L.H. Brush, April 19, 2005. Carlsbad, NM: Sandia National Laboratories. ERMS 539372.

U.S. DOE. 1996a. *Transuranic Waste Baseline Inventory Report, Rev. 3*. DOE/CAO-95-1121. Carlsbad, NM: U.S. Department of Energy Carlsbad Area Office.

U.S. DOE. 1996b. *Title 40 CFR Part 191 Compliance Certification Application for the Waste Isolation Pilot Plant, Vol. 1-21*. DOE/CAO-1994-2184. Carlsbad, NM: U.S. Department of Energy Carlsbad Area Office.

Van Soest, G.D. 2012. *Performance Assessment Inventory Report – 2012, INV-PA-12, Rev. 0*. LA-UR-12-26643. Carlsbad, NM: Los Alamos National Laboratory – Carlsbad Operations.

Van Soest, G.D. 2018. *Performance Assessment Inventory Report – 2018, INV-PA-18, Rev. 0.* LA-UR-18-31882. Carlsbad, NM: Los Alamos National Laboratory – Carlsbad Operations.