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Waste Isolation Pilot Plant

Calculation of Organic Ligand Concentrations for the WIPP Compliance Recertification Application and for Evaluating Assumptions of Waste Homogeneity in WIPP PA

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TABLE OF CONTENTS

1 ABBREVIATIONS, ACRONYMS, ETC. 3

2 REVISION HISTORY 3

3 ESTIMATES OF MASSES 4

4 CALCULATION OF MOLECULAR WEIGHTS 5

5 CALCUALATION OF LIGAND CONCENTRATIONS 6

5.1 Calculations for a Homogeneous Repository 6
5.2 Calculations for a Realistic Panel X 7

5.2.1 Realistic Panel X 7
5.2.2 The Rest of the Repository Associated with a Realistic Panel X 8

5.3 Calculations for a Conservative Panel X 9

5.3.1 Conservative Panel X 9
5.3.2 The Rest of the Repository Associated with a Conservative Panel X 10

5.4 Bounding Cases 12

5.4.1 Panel Filled with IN-BN-510 12
5.4.2 Panel with No IN-BN-510 12

6 CONCULSIONS 13

7 REFERENCES 14

TABLES 1 THROUGH 12 16

1 ABBREVIATIONS, ACRONYMS, ETC.

Table 1 defines the abbreviations, acronyms, etc., used in this report (see page 17).

2 REVISION HISTORY

This analysis report has two objectives: (1) correction of the concentrations of acetate, citrate, ethylenediaminetetraacetate (EDTA), and oxalate (referred to hereafter as "organic ligands" or "ligands" in Waste Isolation Pilot Plant (WIPP) brines for contact-handled (CH) and remote-handled (RH) transuranic (TRU) waste emplaced homogeneously in all 10 panels of the repository, and (2) the first calculations of ligand concentrations in a single panel and the rest of the repository associated with that panel for the analysis by Hansen et al. (2003).

Brush and Xiong (2003a) described their plans for the calculation of actinide solubilities for the performance assessment (PA) for the U.S. Department of Energy's (DOE's) first WIPP Compliance Recertification Application (CRA). Brush and Xiong (2003a, Subsection 7.2, Recalculation of the Concentrations of Organic Ligands) included plans to revise, if necessary, the ligand concentrations estimated for the WIPP Compliance Certification Application (CCA). Brush and Xiong (2003b) used updated estimates of the total masses of ligands to be emplaced in the WIPP from Crawford (2003) to calculate revised ligand concentrations. These concentrations (Brush and Xiong, 2003b, Table 4) replaced those reported by U.S. DOE (1996, Appendix SOTERM, Table SOTERM.5). After Brush and Xiong (2003c) revised their plan for the solubility calculations, Brush and Xiong (2003d) calculated solubilities using the ligand concentrations from Brush and Xiong (2003b).

After these actinide solubilities were used in the first series of PA calculations for the CRA, Crawford and Leigh (2003) and Leigh (2003a) corrected Crawford's (2003) estimates of the total masses of organic ligands to be emplaced in the WIPP. These corrections decreased the masses of ligands in the WIPP inventory. Therefore, the solubilities calculated by Brush and Xiong (2003d) are somewhat higher than those that would be obtained if they were recalculated using the corrected concentrations. The solubilities from Brush and Xiong (2003d) were thus used in the second series of CRA PA calculations.

Meanwhile, Leigh (2003b) estimated the quantities organic ligands in a hypothetical "Panel X" for the analysis by Hansen et al. (2003). The objective of this analysis is to assess the impact of emplacing 100-gal drums of supercompacted waste (waste stream IN-BN-510) from the Advanced Mixed Waste Treatment Project (AMWTP) at the Idaho National Engineering and Environmental Laboratory (INEEL) on the validity of using assumptions of waste homogeneity in WIPP PA. Leigh (2003b) defined two cases for this analysis: (1) a realistic case, in which the portion of the total volume of the CH TRU waste in Panel X occupied by IN-BN-510 is equal to the portion of the total volume of the CH waste in Panel 1 occupied by the largest waste stream in Panel 1, incinerator ash and process residue (waste stream RF 118.01) from the Rocky Flats Environmental Technology Site (RFETS); (2) a conservative case, in which the portion of CH waste containers in Panel X from INEEL is equal to the portion of the containers in Panel 1 from RFETS, the site that shipped the most containers to Panel 1. For both the realistic and the conservative cases, Leigh (2003b) assumed that the ratio of each type of CH waste container with INEEL waste in Panel X to the total quantity of INEEL CH waste containers in Panel X is equal to the ratio of the total quantity of that type of CH waste container to be shipped from INEEL to the total quantity of all the CH waste containers to be shipped from INEEL. Finally, Leigh (2003b) assumed that the total volume of CH waste in Panel X is equal to 1.685×10^5 $m^3 \times 0.1044 = 17{,}591.4$ m^3, in which 1.685×10^5 m^3 is the total volume of CH waste to be emplaced in the WIPP and 0.1044 is the portion of the total WIPP inventory in a seven-room, PA panel (Lappin et al., 1989, Table 4-7).

Leigh (2003b) used the assumptions described above to calculate the following for a realistic and a conservative Panel X: (1) the quantities of INEEL waste containers with IN-BN-510 and with uncompacted waste, and the quantity of containers with waste from all of the other sites; (2) the quantities of organic ligands in each type of container; (3) the total quantities of ligands in Panel X.

This report includes calculations of ligand concentrations for a homogeneous, 10-panel repository, realistic Panel X and the rest of the repository associated with a realistic Panel X, a conservative Panel X and the rest of the repository associated with a conservative Panel X, and two bounding cases for the analysis by Hansen et al. (2003).

We carried out this work under the current version of analysis plan (AP) for the CRA PA solubility calculations (Brush and Xiong, 2003c, Subsection 7.2, Recalculation of the Concentrations of Organic Ligands). Brush and Xiong (2003b) calculated ligand concentrations under the previous version of this AP (Brush and Xiong, 2003a). The revision of this AP did not affect the methods used to calculate ligand concentrations. In fact, the methods used by U.S. DOE (1996, Appendix SOTERM, SOTERM.5), Brush and Xiong (2003b), and the authors of this report are identical, except for the masses of ligands used to calculate concentrations.

3 ESTIMATES OF MASSES

Crawford and Leigh (2003, Table 4, column labeled "Total") provided estimates of the total masses of acetic acid, Na-acetate, citric acid, Na-citrate, Na-EDTA, oxalic acid, and Na-acetate to be emplaced in the WIPP. These estimates have replaced those provided by Crawford (2003, Table 2, column labeled "Scaled Mass (kg)"), which in turn replaced those from U.S. DOE (1996a, Appendix B4), the estimates available at the time of the CCA (U.S. DOE, 1996b, Appendix SOTERM, SOTERM.5).

4 CALCULATION OF MOLECULAR WEIGHTS

We used the following atomic weights to calculate the molecular weights of acetic acid, Na-acetate, citric acid, Na-citrate, Na-EDTA, oxalic acid, and Na-acetate: 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 2 provides the formulas for these compounds.

Acetic acid, citric acid, EDTA, and oxalic acid contain one, three, four, and two protons, respectively, that can be substituted with Na (or other alkali or alkaline-earth metals). Crawford (2003), Crawford and Leigh (2003), and Leigh (2003a, 2003b) did not specify how many of the protons in Na-citrate, Na-EDTA, or Na-oxalate were replaced by Na. Therefore, we assumed that only one of the protons was substituted with Na to calculate the molecular weights of Na-citrate, Na-EDTA, and Na-oxalate. This assumption is "conservative;" in other words, it results in the highest molar quantities of the Na-bearing forms of these ligands.

We calculated the molecular weights of acetic acid, Na-acetate, citric acid, Na-citrate, EDTA (ethylenediaminetetraacetic acid, in this case), Na-EDTA, oxalic acid, and Na-oxalate as follows:

- Acetic acid: (4 × mol wt H) + (2 × mol wt C) + (2 × mol wt 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 × mol wt H) + (2 × mol wt C) + (2 × mol wt O) + (1 × mol wt 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 × mol wt H) + (6 × mol wt C) + (7 × mol wt 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.

- Na-citrate: (7 × mol wt H) + (6 × mol wt C) + (7 × mol wt O) + (1 × mol wt 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 × mol wt H) + (10 × mol wt C) + (2 × mol wt of N) + (8 × mol wt 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.

- Na-EDTA: (15 × mol wt H) + (10 × mol wt C) + (2 × mol wt of N) + (8 × mol wt O) + (1 × mol wt 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 × mol wt H) + (2 × mol wt C) + (4 × mol wt 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.

- Na-oxalate: (1 × mol wt H) + (2 × mol wt C) + (4 × mol wt O) + (1 × mol wt 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 2 provides the results of these calculations (see page 18).

5 CALCUALATION OF LIGAND CONCENTRATIONS

5.1 Calculations for a Homogeneous Repository

We used 29,841 m^3 of brine, "the smallest quantity of brine required to be in the repository [for] transport away from the repository" (Larson, 1996; U.S. DOE, 1996b), to calculate the dissolved concentrations of acetate, citrate, EDTA, and oxalate in a homogeneous, 10-panel PA repository. This volume is conservative because any volume greater than 29,841 m^3 would result in lower concentrations of these ligands. A volume of 29,841 m^3 of brine is equivalent to 29,841,000 L of brine.

We calculated the concentrations of acetic acid, Na-acetate, citric acid, Na-citrate, Na-EDTA, oxalic acid, and Na-oxalate by multiplying the total masses of these compounds in kg from Crawford and Leigh (2003, Table 4, column labeled "Total Mass") by 1000 g/kg to convert Crawford and Leigh's estimates to total masses in grams. Next, we divided these masses by the molecular weights of these compounds from Table 2 of this report, column labeled "Mol Wt (g)," which yielded the total quantities of these compounds to be emplaced in mol. We then divided these quantities by 29,841,000 L to obtain the concentrations of these compounds in units of mol/L (M):

- Acetic acid: $((1.42 \times 10^2\ \text{kg}) \times (1000\ \text{g/kg}) \div (60.0520\ \text{g/mol})) \div 2.9841 \times 10^7\ \text{L} = 7.92 \times 10^{-5}\ \text{M}$.

- Na-acetate: $((8.51 \times 10^3 \text{ kg}) \times (1000 \text{ g/kg}) \div (82.0338 \text{ g/mol})) \div 2.9841 \times 10^7 \text{ L} = 3.48 \times 10^{-3}$ M.

- Citric acid: $((1.19 \times 10^3 \text{ kg}) \times (1000 \text{ g/kg}) \div (192.1235 \text{ g/mol})) \div 2.9841 \times 10^7 \text{ L} = 2.08 \times 10^{-4}$ M.

- Na-citrate: $((4.00 \times 10^2 \text{ kg}) \times (1000 \text{ g/kg}) \div (214.1054 \text{ g/mol})) \div 2.9841 \times 10^7 \text{ L} = 6.26 \times 10^{-5}$ M.

- Na-EDTA: $((2.56 \times 10^1 \text{ kg}) \times (1000 \text{ g/kg}) \div (314.2246 \text{ g/mol})) \div 2.9841 \times 10^7 \text{ L} = 2.73 \times 10^{-6}$ M.

- Oxalic acid: $((1.38 \times 10^4 \text{ kg}) \times (1000 \text{ g/kg}) \div (90.0349 \text{ g/mol})) \div 2.9841 \times 10^7 \text{ L} = 5.14 \times 10^{-3}$ M.

- Na-oxalate: $((3.39 \times 10^4 \text{ kg}) \times (1000 \text{ g/kg}) \div (112.0167 \text{ g/mol})) \div 2.9841 \times 10^7 \text{ L} = 1.02 \times 10^{-2}$ M.

Table 3 summarizes these calculations and provides the results (see page 19).

We calculated the total dissolved concentrations of acetate, citrate, and oxalate by adding the concentrations of acetic acid and Na-acetate, citric acid and Na-citrate, and oxalic acid and Na-oxalate. The concentration of Na-EDTA is equal to the total concentration of EDTA because Crawford and Leigh (2003) did not report any EDTA without Na. Table 4 (see page 20) provides the corrected total dissolved concentrations of acetate, citrate, EDTA, and oxalate for a homogeneous, 10-panel repository and compares them to the concentrations calculated by Brush and Xiong (2003d) for a homogeneous, 10-panel repository for the CRA PA.

5.2 Calculations for a Realistic Panel X

5.2.1 Realistic Panel X

We used 29,841 m^3 of brine × 0.1044 = 3115.4 m^3 of brine, in which 29,841 m^3 is "the smallest quantity of brine required to be in the repository [for] transport away from the repository" (Larson, 1996; U.S. DOE, 1996b) and 0.1044 is the portion of the total WIPP inventory in a seven-room, PA panel (Lappin et al., 1989, Table 4-7), to calculate the dissolved concentrations of acetate, citrate, EDTA, and oxalate in a realistic Panel X loaded with the same quantity of waste as a seven-room, PA panel. A volume of 3,115.4 m^3 of brine is equivalent to 3,115,400 L of brine.

We calculated the concentrations of acetic acid, Na-acetate, citric acid, Na-citrate, Na-EDTA, oxalic acid, and Na-oxalate by multiplying the total masses of these compounds in kg from Leigh (2003b, Table 7, row labeled "Panel X" under

"Realistic Case") by 1000 g/kg to convert Leigh's estimates to total masses in grams. Next, we divided these masses by the molecular weights of these compounds from Table 2 of this report, which yielded the total quantities of these compounds to be emplaced in mol. We then divided these quantities by 3,115,400 L to obtain the concentrations of these compounds in M:

- Acetic acid: $((1.44 \times 10^1$ kg$) \times (1000$ g/kg$) \div (60.0520$ g/mol$)) \div 3.1154 \times 10^6$ L $= 7.70 \times 10^{-5}$ M.
- Na-acetate: $((8.63 \times 10^2$ kg$) \times (1000$ g/kg$) \div (82.0338$ g/mol$)) \div 3.1154 \times 10^6$ L $= 3.38 \times 10^{-3}$ M.
- Citric acid: $((1.21 \times 10^2$ kg$) \times (1000$ g/kg$) \div (192.1235$ g/mol$)) \div 3.1154 \times 10^6$ L $= 2.02 \times 10^{-4}$ M.
- Na-citrate: $((4.06 \times 10^1$ kg$) \times (1000$ g/kg$) \div (214.1054$ g/mol$)) \div 3.1154 \times 10^6$ L $= 6.09 \times 10^{-5}$ M.
- Na-EDTA: $((2.60 \times 10^0$ kg$) \times (1000$ g/kg$) \div (314.2246$ g/mol$)) \div 3.1154 \times 10^6$ L $= 2.66 \times 10^{-6}$ M.
- Oxalic acid: $((1.40 \times 10^3$ kg$) \times (1000$ g/kg$) \div (90.0349$ g/mol$)) \div 3.1154 \times 10^6$ L $= 4.99 \times 10^{-3}$ M.
- Na-oxalate: $((3.44 \times 10^3$ kg$) \times (1000$ g/kg$) \div (112.0167$ g/mol$)) \div 3.1154 \times 10^6$ L $= 9.86 \times 10^{-3}$ M.

Table 5 summarizes these calculations (see page 21).

5.2.2 The Rest of the Repository Associated with a Realistic Panel X

We used 29,841 m^3 of brine $\times$ 0.8956 = 26,725.6 m^3 of brine, in which 29,841 m^3 is "the smallest quantity of brine required to be in the repository [for] transport away from the repository" (Larson, 1996; U.S. DOE, 1996b) and 0.8956 is the portion of the total WIPP inventory in seven seven-room, PA panels and the northern and southern equivalent panels (Lappin et al., 1989, Table 4-7), to calculate the dissolved concentrations of acetate, citrate, EDTA, and oxalate in the rest of the repository associated with a realistic Panel X. A volume of 26,725.6 m^3 of brine is equivalent to 26,725,600 L of brine.

We calculated the concentrations of acetic acid, Na-acetate, citric acid, Na-citrate, Na-EDTA, oxalic acid, and Na-oxalate by multiplying the total masses of these compounds in kg from Leigh (2003b, Table 7, row labeled "Rest of Repository" under "Realistic Case") by 1000 g/kg to convert Leigh's estimates to total masses in grams. Next, we divided these masses by the molecular weights of these compounds from

Table 2 of this report, which yielded the total quantities of these compounds to be emplaced in mol. We then divided these quantities by 26,725,600 L to obtain the concentrations of these compounds in M:

- Acetic acid: $((1.28 \times 10^2\ \text{kg}) \times (1000\ \text{g/kg}) \div (60.0520\ \text{g/mol})) \div 2.67256 \times 10^7\ \text{L} = 7.98 \times 10^{-5}\ \text{M}$.

- Na-acetate: $((7.65 \times 10^3\ \text{kg}) \times (1000\ \text{g/kg}) \div (82.0338\ \text{g/mol})) \div 2.67256 \times 10^7\ \text{L} = 3.49 \times 10^{-3}\ \text{M}$.

- Citric acid: $((1.07 \times 10^3\ \text{kg}) \times (1000\ \text{g/kg}) \div (192.1235\ \text{g/mol})) \div 2.67256 \times 10^7\ \text{L} = 2.08 \times 10^{-4}\ \text{M}$.

- Na-citrate: $((3.59 \times 10^2\ \text{kg}) \times (1000\ \text{g/kg}) \div (214.1054\ \text{g/mol})) \div 2.67256 \times 10^7\ \text{L} = 6.27 \times 10^{-5}\ \text{M}$.

- Na-EDTA: $((2.30 \times 10^1\ \text{kg}) \times (1000\ \text{g/kg}) \div (314.2246\ \text{g/mol})) \div 2.67256 \times 10^7\ \text{L} = 2.74 \times 10^{-6}\ \text{M}$.

- Oxalic acid: $((1.24 \times 10^4\ \text{kg}) \times (1000\ \text{g/kg}) \div (90.0349\ \text{g/mol})) \div 2.67256 \times 10^7\ \text{L} = 5.15 \times 10^{-3}\ \text{M}$.

- Na-oxalate: $((3.05 \times 10^4\ \text{kg}) \times (1000\ \text{g/kg}) \div (112.0167\ \text{g/mol})) \div 2.67256 \times 10^7\ \text{L} = 1.02 \times 10^{-2}\ \text{M}$.

Table 6 summarizes these calculations (see page 22).

We calculated the total dissolved concentrations of acetate, citrate, and oxalate by adding the concentrations of acetic acid and Na-acetate, citric acid and Na-citrate, and oxalic acid and Na-oxalate in Tables 5 and 6. The concentration of Na-EDTA is equal to the total concentration of EDTA because Leigh (2003b) did not report any EDTA without Na. Table 7 (see page 23) provides the total dissolved concentrations of acetate, citrate, EDTA, and oxalate for a realistic Panel X the rest of the repository associated with it, and compares them to the concentrations for a homogeneous, 10-panel repository calculated by Brush and Xiong (2003d) for the CRA PA and the corrected concentrations for a homogeneous, 10-panel calculated for this report.

5.3 Calculations for a Conservative Panel X

5.3.1 Conservative Panel X

We used 29,841 m^3 of brine $\times$ 0.1044 = 3115.4 m^3 of brine, in which 29,841 m^3 is "the smallest quantity of brine required to be in the repository [for] transport away from the repository" (Larson, 1996; U.S. DOE, 1996b) and 0.1044 is the portion of the total

WIPP inventory in a seven-room, PA panel (Lappin et al., 1989, Table 4-7), to calculate the dissolved concentrations of acetate, citrate, EDTA, and oxalate in a realistic Panel X loaded with the same quantity of waste as a seven-room, PA panel. A volume of 3,115.4 m^3 of brine is equivalent to 3,115,400 L of brine.

We calculated the concentrations of acetic acid, Na-acetate, citric acid, Na-citrate, Na-EDTA, oxalic acid, and Na-oxalate by multiplying the total masses of these compounds in kg from Leigh (2003b, Table 7, row labeled "Panel X" under "Conservative Case") by 1000 g/kg to convert Leigh's estimates to total masses in grams. Next, we divided these masses by the molecular weights of these compounds from Table 2 of this report, which yielded the total quantities of these compounds to be emplaced in mol. We then divided these quantities by 3,115,400 L to obtain the concentrations of these compounds in M:

- Acetic acid: $((1.20 \times 10^1 \text{ kg}) \times (1000 \text{ g/kg}) \div (60.0520 \text{ g/mol})) \div 3.1154 \times 10^6 \text{ L} = 6.41 \times 10^{-5}$ M.

- Na-acetate: $((7.19 \times 10^2 \text{ kg}) \times (1000 \text{ g/kg}) \div (82.0338 \text{ g/mol})) \div 3.1154 \times 10^6 \text{ L} = 2.81 \times 10^{-3}$ M.

- Citric acid: $((1.01 \times 10^2 \text{ kg}) \times (1000 \text{ g/kg}) \div (192.1235 \text{ g/mol})) \div 3.1154 \times 10^6 \text{ L} = 1.69 \times 10^{-4}$ M.

- Na-citrate: $((3.38 \times 10^1 \text{ kg}) \times (1000 \text{ g/kg}) \div (214.1054 \text{ g/mol})) \div 3.1154 \times 10^6 \text{ L} = 5.07 \times 10^{-5}$ M.

- Na-EDTA: $((2.16 \times 10^0 \text{ kg}) \times (1000 \text{ g/kg}) \div (314.2246 \text{ g/mol})) \div 3.1154 \times 10^6 \text{ L} = 2.21 \times 10^{-6}$ M.

- Oxalic acid: $((1.16 \times 10^3 \text{ kg}) \times (1000 \text{ g/kg}) \div (90.0349 \text{ g/mol})) \div 3.1154 \times 10^6 \text{ L} = 4.14 \times 10^{-3}$ M.

- Na-oxalate: $((2.87 \times 10^3 \text{ kg}) \times (1000 \text{ g/kg}) \div (112.0167 \text{ g/mol})) \div 3.1154 \times 10^6 \text{ L} = 8.22 \times 10^{-3}$ M.

Table 8 summarizes these calculations (see page 24).

5.3.2 The Rest of the Repository Associated with a Conservative Panel X

We used 29,841 m^3 of brine × 0.8956 = 26,725.6 m^3 of brine, in which 29,841 m^3 is "the smallest quantity of brine required to be in the repository [for] transport away from the repository" (Larson, 1996; U.S. DOE, 1996b) and 0.8956 is the portion of the total WIPP inventory in seven seven-room, PA panels and the northern and southern equivalent panels (Lappin et al., 1989, Table 4-7), to calculate the dissolved concentrations of acetate, citrate, EDTA, and oxalate in the rest of the repository associated with a conservative Panel X. A volume of 26,725.6 m^3 of brine is equivalent to 26,725,600 L of brine.

We calculated the concentrations of acetic acid, Na-acetate, citric acid, Na-citrate, Na-EDTA, oxalic acid, and Na-oxalate by multiplying the total masses of these compounds in kg from Leigh (2003b, Table 7, row labeled "Rest of Repository" under "Conservative Case") by 1000 g/kg to convert Leigh's estimates to total masses in grams. Next, we divided these masses by the molecular weights of these compounds from Table 2 of this report, which yielded the total quantities of these compounds to be emplaced in mol. We then divided these quantities by 26,725,600 L to obtain the concentrations of these compounds in M:

- Acetic acid: $((1.30 \times 10^2 \text{ kg}) \times (1000 \text{ g/kg}) \div (60.0520 \text{ g/mol})) \div 2.67256 \times 10^7 \text{ L} = 8.10 \times 10^{-5}$ M.
- Na-acetate: $((7.79 \times 10^3 \text{ kg}) \times (1000 \text{ g/kg}) \div (82.0338 \text{ g/mol})) \div 2.67256 \times 10^7 \text{ L} = 3.55 \times 10^{-3}$ M.
- Citric acid: $((1.09 \times 10^3 \text{ kg}) \times (1000 \text{ g/kg}) \div (192.1235 \text{ g/mol})) \div 2.67256 \times 10^7 \text{ L} = 2.12 \times 10^{-4}$ M.
- Na-citrate: $((3.66 \times 10^2 \text{ kg}) \times (1000 \text{ g/kg}) \div (214.1054 \text{ g/mol})) \div 2.67256 \times 10^7 \text{ L} = 6.40 \times 10^{-5}$ M.
- Na-EDTA: $((2.34 \times 10^1 \text{ kg}) \times (1000 \text{ g/kg}) \div (314.2246 \text{ g/mol})) \div 2.67256 \times 10^7 \text{ L} = 2.79 \times 10^{-6}$ M.
- Oxalic acid: $((1.26 \times 10^4 \text{ kg}) \times (1000 \text{ g/kg}) \div (90.0349 \text{ g/mol})) \div 2.67256 \times 10^7 \text{ L} = 5.24 \times 10^{-3}$ M.
- Na-oxalate: $((3.11 \times 10^4 \text{ kg}) \times (1000 \text{ g/kg}) \div (112.0167 \text{ g/mol})) \div 2.67256 \times 10^7 \text{ L} = 1.04 \times 10^{-2}$ M.

Table 9 summarizes these calculations (see page 25).

We calculated the total dissolved concentrations of acetate, citrate, and oxalate by adding the concentrations of acetic acid and Na-acetate, citric acid and Na-citrate, and oxalic acid and Na-oxalate in Tables 8 and 9. The concentration of Na-EDTA is equal to the total concentration of EDTA because Leigh (2003b) did not report any EDTA without Na. Table 10 (see page 26) provides the total dissolved concentrations of acetate, citrate, EDTA, and oxalate for a conservative Panel X and the rest of the repository associated with it, and compares them to the concentrations for a homogeneous, 10-panel repository calculated by Brush and Xiong (2003d) for the CRA PA and the corrected concentrations for a homogeneous, 10-panel repository calculated for this report.

5.4 Bounding Cases

5.4.1 Panel Filled with IN-BN-510

IN-BN-510 contains no ligands (Leigh, 2003b). Therefore, any brine in a panel filled entirely with IN-BN-510 would have ligand concentrations of 0.

5.4.2 CH Waste with No IN-BN-510

We used 29,841 m^3 of brine $\times$ 0.882 = 26,321 m^3 of brine, in which 29,841 m^3 is "the smallest quantity of brine required to be in the repository [for] transport away from the repository" (Larson, 1996; U.S. DOE, 1996b) and 0.882 is the portion of the CH inventory remaining after subtracting the total volume of 19,875 m^3 of IN-BN-510 waste from the total CH-waste inventory of 168,500 m^3, to calculate the dissolved concentrations of acetate, citrate, EDTA, and oxalate for CH waste without any ligand-free IN-BN-510 present. Because IN-BN-510 contains no ligands, so subtraction of this waste stream prevents any dilution of the waste that does contain ligands with ligand-free waste. We obtained 19,875 by multiplying 52,440 drums of IN-BN-510, the total number of drums containing IN-BN-510 waste that will eventually be shipped from INEEL, by 0.379 m^3, the volume of a 100-gal drum (Leigh, 2003b). A volume of 26,321 m^3 of brine is equivalent to 26,321,000 L of brine.

We calculated the concentrations of acetic acid, Na-acetate, citric acid, Na-citrate, Na-EDTA, oxalic acid, and Na-oxalate by multiplying the total masses of these compounds in kg from Crawford and Leigh (2003, Table 4, column labeled "Total Mass") by 1000 g/kg to convert Crawford and Leigh's estimates to total masses in grams. Next, we divided these masses by the molecular weights of these compounds from Table 2 of this report, which yielded the total quantities of these compounds to be emplaced in mol. We then divided these quantities by 26,321,000 L to obtain the concentrations of these compounds in M:

- Acetic acid: $((1.42 \times 10^2 \text{ kg}) \times (1000 \text{ g/kg}) \div (60.0520 \text{ g/mol})) \div 2.6321 \times 10^7 \text{ L} = 8.98 \times 10^{-5}$ M.

- Na-acetate: $((8.51 \times 10^3 \text{ kg}) \times (1000 \text{ g/kg}) \div (82.0338 \text{ g/mol})) \div 2.6321 \times 10^7 \text{ L} = 3.94 \times 10^{-3}$ M.

- Citric acid: $((1.19 \times 10^3 \text{ kg}) \times (1000 \text{ g/kg}) \div (192.1235 \text{ g/mol})) \div 22.6321 \times 10^7 \text{ L} = 2.35 \times 10^{-4}$ M.

- Na-citrate: $((4.00 \times 10^2 \text{ kg}) \times (1000 \text{ g/kg}) \div (214.1054 \text{ g/mol})) \div 2.6321 \times 10^7 \text{ L} = 7.10 \times 10^{-5}$ M.

- Na-EDTA: ((2.56 × 10^1 kg) × (1000 g/kg) ÷ (314.2246 g/mol)) ÷ 2.6321 ×10^7 L = 3.10 × 10^{-6} M.

- Oxalic acid: ((1.38 × 10^4 kg) × (1000 g/kg) ÷ (90.0349 g/mol)) ÷ 2.6321 ×10^7 L = 5.82 × 10^{-3} M.

- Na-oxalate: ((3.39 × 10^4 kg) × (1000 g/kg) ÷ (112.0167 g/mol)) ÷ 2.6321 ×10^7 L = 1.15 × 10^{-2} M.

Table 11 summarizes these calculations (see page 27).

We calculated the total dissolved concentrations of acetate, citrate, and oxalate by adding the concentrations of acetic acid and Na-acetate, citric acid and Na-citrate, and oxalic acid and Na-oxalate in Table 11. The concentration of Na-EDTA is equal to the total concentration of EDTA because Crawford and Leigh (2003) did not report any EDTA without Na. Table 12 (see page 28) provides the total dissolved concentrations of acetate, citrate, EDTA, and oxalate for a bounding case with a panel that contains all IN-BN-510 and a bounding case that contains no IN-BN-510, and compares them to the concentrations for a homogeneous, 10-panel repository calculated by Brush and Xiong (2003d) for the CRA PA and the corrected concentrations for a homogeneous, 10-panel repository calculated for this report.

6 CONCULSIONS

The results of this analysis demonstrate that – in every case considered for the analysis of Hansen et al. (2003), including a homogeneous, 10-panel repository; a hypothetical Panel X with realistic and conservative loadings of AMWTP waste; the rest of the repository associated with Panel X; and two bounding cases – the concentrations of acetate, citrate, EDTA, and oxalate in WIPP brines are less than those used by Brush and Xiong (2003d) to calculate actinide solubilities for the CRA PA.

The main reason for this conclusion is that the corrected, updated masses of ligands in the WIPP inventory from Crawford and Leigh (2003) are only 70.5% of the original, updated masses from Crawford (2003), who scaled up the masses reported by the TRU-waste generator sites despite the fact all of the ligands are in the category referred to as "Stored Waste," a category that is not scaled up when the "Projected" CH waste is scaled to ensure that the total volume of CH waste will be 1.685 × 10^5 m^3. Leigh (2003a) provided a detailed explanation of the inappropriateness of scaling up the masses of ligands to be emplaced in the WIPP.

However, it is also apparent that, because IN-BN-510 contains no organic ligands at all, any preferential loading of this waste stream in a WIPP panel (or panels) will result in lower ligand concentrations in that panel or panels.

Therefore, the solubilities calculated by Brush and Xiong (2003d) for the first series of CRA PA calculations - which used Brush and Xiong's (2003b) ligand concentrations, based on the uncorrected estimates of ligand masses from Crawford (2003) - are somewhat higher than those that would be obtained if they were recalculated using the corrected concentrations from this report, based on the corrected masses of Crawford and Leigh (2003) and Leigh (2003a). The solubilities from Brush and Xiong (2003d) were thus used in the second series of CRA PA calculations and for the analysis of Hansen et al. (2003).

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TABLES 1 THROUGH 12

Table 1. Abbreviations, Acronyms, etc.

Abbreviation, Acronym, etc.	Definition
acetate	$CH_3CO_2^+$
acetic acid	CH_3CO_2H
AMWTP	Advanced Mixed Waste Treatment Project
DOE	(U.S.) Department of Energy
C	carbon
CCA	(WIPP) Compliance Certification Application
citrate	$(CH_2CO_2H)_2C(OH)(CO_2)^+$
citric acid	$(CH_2CO_2H)_2C(OH)(CO_2H)$
CRA	(WIPP) Compliance Recertification Application
EDTA	ethylenediaminetetraacetate, $(CH_2CO_2H)_2N(CH_2)_2N(CH_2CO_2H)(CH_2CO_2)^+$; or ethylenediaminetetraacetic acid, $(CH_2CO_2H)_2N(CH_2)_2N(CH_2CO_2H)_2$
g	gram(s)
gal	gallon(s)
H	hydrogen
IN-BN-510	the AMWTP supercompacted waste stream
INEEL	Idaho National Engineering and Environmental Laboratory
kg	kilogram(s)
L	liter(s)
M	molar
m	meter(s) or molal
mol	moles
N	nitrogen
Na	sodium
Na-acetate	CH_3CO_2Na
Na-citrate	$(CH_2CO_2H)_2C(OH)(CO_2Na)$
Na-EDTA	$(CH_2CO_2H)_2N(CH_2)_2N(CH_2CO_2H)(CH_2CO_2Na)$
Na-oxalate	$(CO_2H)(CO_2Na)$
O	oxygen
oxalate	$(CO_2H)(CO_2)^+$
oxalic acid	$(CO_2H)_2$
PA	performance assessment
RFETS	Rocky Flats Environmental Technology Site
WIPP	(U.S. DOE) Waste Isolation Pilot Plant
wt	weight

Table 2. Formulas and Molecular Weights of Two Forms of Four Ligands That Could Be Emplaced in the WIPP.

Compound	Formula	Mol Wt (g)
Acetic acid	CH_3CO_2H	60.0520
Na-acetate	CH_3CO_2Na	82.0338
Citric acid	$(CH_2CO_2H)_2C(OH)(CO_2H)$	192.1235
Na-citrate	$(CH_2CO_2H)_2C(OH)(CO_2Na)$	214.1054
EDTA	$(CH_2CO_2H)_2N(CH_2)_2N(CH_2CO_2H)_2$	292.2427
Na-EDTA	$(CH_2CO_2H)_2N(CH_2)_2N(CH_2CO_2H)(CH_2CO_2Na)$	314.2246
Oxalic acid	$(CO_2H)_2$	90.0349
Na-oxalate	$(CO_2H)(CO_2Na)$	112.0167

Table 3. Dissolved Concentrations of One or Two Forms of Four Ligands for a Homogeneous, 10-Panel Repository.

Compound	Total Mass (kg)[A]	Total Mass (g)	Total Quantity (mol)	Concentration (M)
Acetic acid	1.42×10^{2}	1.42×10^{5}	2.36×10^{3}	7.92×10^{-5}
Na-acetate	8.51×10^{3}	8.51×10^{6}	1.04×10^{5}	3.48×10^{-3}
Citric acid	1.19×10^{3}	1.19×10^{6}	6.20×10^{3}	2.08×10^{-4}
Na-citrate	4.00×10^{2}	4.00×10^{5}	1.87×10^{3}	6.26×10^{-5}
Na-EDTA	2.56×10^{1}	2.56×10^{4}	8.15×10^{1}	2.73×10^{-6}
Oxalic acid	1.38×10^{4}	1.38×10^{7}	1.53×10^{5}	5.14×10^{-3}
Na-oxalate	3.39×10^{4}	3.39×10^{7}	3.03×10^{5}	1.02×10^{-2}

A. From Crawford and Leigh (2003, Table 4, column labeled "Total Mass").

Table 4. Total Concentrations of Four Ligands for a Homogeneous, 10-Panel Repository.

Ligand	Concentration for a 10-Panel, Homogeneous Repository (M), Brush and Xiong (2003d)[A]	Corrected Concentration for a 10-Panel, Homogeneous Repository (M), This Report
Acetate	5.05×10^{-3}	3.56×10^{-3}
Citrate	3.83×10^{-4}	2.71×10^{-4}
EDTA	3.87×10^{-6}	2.73×10^{-6}
Oxalate	2.16×10^{-2}	1.53×10^{-2}

A. Concentrations used to calculate solubilities for the CRA PA.

Table 5. Dissolved Concentrations of One or Two Forms of Four Ligands for a Realistic Panel X.

Compound	Total Mass (kg)[A]	Total Mass (g)	Total Quantity (mol)	Concentration (M)
Acetic acid	1.44×10^{1}	1.44×10^{4}	2.40×10^{2}	7.70×10^{-5}
Na-acetate	8.63×10^{2}	8.63×10^{5}	1.05×10^{4}	3.38×10^{-3}
Citric acid	1.21×10^{2}	1.21×10^{5}	6.30×10^{2}	2.02×10^{-4}
Na-citrate	4.06×10^{1}	4.06×10^{4}	1.90×10^{2}	6.09×10^{-5}
Na-EDTA	2.60×10^{0}	2.60×10^{3}	8.27×10^{0}	2.66×10^{-6}
Oxalic acid	1.40×10^{3}	1.40×10^{6}	1.55×10^{4}	4.99×10^{-3}
Na-oxalate	3.44×10^{3}	3.44×10^{6}	3.07×10^{4}	9.86×10^{-3}

A. From Leigh (2003d, Table 7, row labeled "Panel X" under "Realistic Case").

Table 6. Dissolved Concentrations of One or Two Forms of Four Ligands for the Rest of the Repository Associated with a Realistic Panel X.

Compound	Total Mass (kg)[A]	Total Mass (g)	Total Quantity (mol)	Concentration (M)
Acetic acid	1.28×10^{2}	1.28×10^{5}	2.13×10^{3}	7.98×10^{-5}
Na-acetate	7.65×10^{3}	7.65×10^{6}	9.33×10^{4}	3.49×10^{-3}
Citric acid	1.07×10^{3}	1.07×10^{6}	5.57×10^{3}	2.08×10^{-4}
Na-citrate	3.59×10^{2}	3.59×10^{5}	1.68×10^{3}	6.27×10^{-5}
Na-EDTA	2.30×10^{1}	2.30×10^{4}	7.32×10^{1}	2.74×10^{-6}
Oxalic acid	1.24×10^{4}	1.24×10^{7}	1.38×10^{5}	5.15×10^{-3}
Na-oxalate	3.05×10^{4}	3.05×10^{7}	2.72×10^{5}	1.02×10^{-2}

A. From Leigh (2003d, Table 7, row labeled "Rest of Repository" under "Realistic Case").

Table 7. Total Concentrations of Four Ligands for a Homogeneous, 10-Panel Repository, a Realistic Panel X, and the Rest of the Repository Associated with a Realistic Panel X.

Ligand	Concentration for a 10-Panel, Homogeneous Repository (M), Brush and Xiong (2003d)[A]	Corrected Concentration for a 10-Panel, Homogeneous Repository (M), This Report	Concentration for a Realistic Panel X (M), This Report	Concentration for the Rest of Repository Assoc. with a Realistic Panel X (M), This Report
Acetate	5.05×10^{-3}	3.56×10^{-3}	3.46×10^{-3}	3.57×10^{-3}
Citrate	3.83×10^{-4}	2.71×10^{-4}	2.63×10^{-4}	2.71×10^{-4}
EDTA	3.87×10^{-6}	2.73×10^{-6}	2.66×10^{-6}	2.74×10^{-6}
Oxalate	2.16×10^{-2}	1.53×10^{-2}	1.48×10^{-2}	1.54×10^{-2}

A. Concentrations used to calculate solubilities for the CRA PA.

Table 8. Dissolved Concentrations of One or Two Forms of Four Ligands for a Conservative Panel X.

Compound	Total Mass (kg)[A]	Total Mass (g)	Total Quantity (mol)	Concentration (M)
Acetic acid	1.20×10^{1}	1.20×10^{4}	2.00×10^{2}	6.41×10^{-5}
Na-acetate	7.19×10^{2}	7.19×10^{5}	8.76×10^{3}	2.81×10^{-3}
Citric acid	1.01×10^{2}	1.01×10^{5}	5.26×10^{2}	1.69×10^{-4}
Na-citrate	3.38×10^{1}	3.38×10^{4}	1.58×10^{2}	5.07×10^{-5}
Na-EDTA	2.16×10^{0}	2.16×10^{3}	6.87×10^{0}	2.21×10^{-6}
Oxalic acid	1.16×10^{3}	1.16×10^{6}	1.29×10^{4}	4.14×10^{-3}
Na-oxalate	2.87×10^{3}	2.87×10^{6}	2.56×10^{4}	8.22×10^{-3}

A. From Leigh (2003d, Table 7, row labeled "Panel X" under "Conservative Case").

Table 9. Dissolved Concentrations of One or Two Forms of Four Ligands for the Rest of the Repository Associated with a Conservative Panel X.

Compound	Total Mass (kg)[A]	Total Mass (g)	Total Quantity (mol)	Concentration (M)
Acetic acid	1.30×10^{2}	1.30×10^{5}	2.16×10^{3}	8.10×10^{-5}
Na-acetate	7.79×10^{3}	7.79×10^{6}	9.50×10^{4}	3.55×10^{-3}
Citric acid	1.09×10^{3}	1.09×10^{6}	5.67×10^{3}	2.12×10^{-4}
Na-citrate	3.66×10^{2}	3.66×10^{5}	1.71×10^{3}	6.40×10^{-5}
Na-EDTA	2.34×10^{1}	2.34×10^{4}	7.45×10^{1}	2.79×10^{-6}
Oxalic acid	1.26×10^{4}	1.26×10^{7}	1.40×10^{5}	5.24×10^{-3}
Na-oxalate	3.11×10^{4}	3.11×10^{7}	2.78×10^{5}	1.04×10^{-2}

A. From Leigh (2003d, Table 7, row labeled "Rest of Repository" under "Conservative Case").

Table 10. Total Concentrations of Four Ligands for a Homogeneous, 10-Panel Repository, a Realistic Panel X, and the Rest of the Repository Associated with a Realistic Panel X.

Ligand	Concentration for a 10-Panel, Homogeneous Repository (M), Brush and Xiong (2003d)[A]	Corrected Concentration for a 10-Panel, Homogeneous Repository (M), This Report	Concentration for a Conservative Panel X (M), This Report	Concentration for the Rest of Repository Assoc. with a Conservative Panel X (M), This Report
Acetate	5.05×10^{-3}	3.56×10^{-3}	2.87×10^{-3}	3.63×10^{-3}
Citrate	3.83×10^{-4}	2.71×10^{-4}	2.20×10^{-4}	2.76×10^{-4}
EDTA	3.87×10^{-6}	2.73×10^{-6}	2.21×10^{-6}	2.79×10^{-6}
Oxalate	2.16×10^{-2}	1.53×10^{-2}	1.24×10^{-2}	1.56×10^{-2}

A. Concentrations used to calculate solubilities for the CRA PA.

Table 11. Dissolved Concentrations of One or Two Forms of Four Ligands for the Bounding Case with a Panel that Contains No IN-BN-510.

Compound	Total Mass (kg)[A]	Total Mass (g)	Total Quantity (mol)	Concentration (M)
Acetic acid	1.42×10^{2}	1.42×10^{5}	2.36×10^{3}	8.98×10^{-5}
Na-acetate	8.51×10^{3}	8.51×10^{6}	1.04×10^{5}	3.94×10^{-3}
Citric acid	1.19×10^{3}	1.19×10^{6}	6.20×10^{3}	2.35×10^{-4}
Na-citrate	4.00×10^{2}	4.00×10^{5}	1.87×10^{3}	7.10×10^{-5}
Na-EDTA	2.56×10^{1}	2.56×10^{4}	8.15×10^{1}	3.10×10^{-6}
Oxalic acid	1.38×10^{4}	1.38×10^{7}	1.53×10^{5}	5.82×10^{-3}
Na-oxalate	3.39×10^{4}	3.39×10^{7}	3.03×10^{5}	1.15×10^{-2}

A. From Crawford and Leigh (2003, Table 4, column labeled "Total Mass").

Table 12. Total Concentrations of Four Ligands for a Homogeneous, 10-Panel Repository, a Bounding Case with a Panel That Contains All IN-BN-510, and a Bounding Case with a Panel That Contains No IN-BN-510.

Ligand	Concentration for a 10-Panel, Homogeneous Repository (M), Brush and Xiong (2003d)[A]	Corrected Concentration for a 10-Panel, Homogeneous Repository (M), This Report	Concentration for a Bounding Case with a Panel That Contains All IN-BN-510 (M)	Concentration for a Bounding Case with a Panel That Contains No IN-BN-510 (M)
Acetate	5.05×10^{-3}	3.56×10^{-3}	0	4.08×10^{-3}
Citrate	3.83×10^{-4}	2.71×10^{-4}	0	2.99×10^{-4}
EDTA	3.87×10^{-6}	2.73×10^{-6}	0	3.10×10^{-6}
Oxalate	2.16×10^{-2}	1.53×10^{-2}	0	1.73×10^{-2}

A. Concentrations used to calculate solubilities for the CRA PA.