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Waste Isolation Pilot Plant

Sensitivity of the Long-Term Performance of The WIPP to EDTA

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1 INTRODUCTION

This analysis report describes a study of the effects of the dissolved concentration of ethylenediaminetetraacetate (EDTA) in repository brines on the long-term performance of the WIPP with respect to the release limits specified by the EPA in Section 191.13 of its containment requirements for radioactive waste (U.S. EPA, 1985; 1993).

SNL's PA staff will use the results of this analysis to assess the impact on performance, if any, of a possible increase in the quantity of EDTA in the inventory of the transuranic (TRU) waste to be emplaced in the WIPP. Los Alamos National Laboratory – Carlsbad Operations (LANL – CO) staff are preparing the TRU waste inventory report for 2007 at this time; the DOE's Carlsbad Field Office will issue it sometime in 2008.

The remainder of this section summarizes the methods used for the speciation and solubility calculations and the PA calculations for this analysis (Subsection 1.1), describes the analysis plan (AP) under which this study was carried out (Subsection 1.2), and provides information on the software used for this analysis (Subsection 1.3).

1.1 Summary of Calculations

For this sensitivity analysis, we used the code FMT (Babb and Novak, 1997 and addenda; Wang, 1998) to calculate the speciation and solubilities of actinide (An) elements in the +III, +IV, and +V oxidation states (An(III), An(IV), and An(V)) in WIPP brines. We used the same conceptual models, parameters, and code that were used to calculate these solubilities for the first WIPP Compliance Recertification Application (CRA-2004) Performance Assessment Baseline Calculations (PABC), except with EDTA concentrations 10 times and 100 times that used for the CRA-2004 PABC.

We then used the WIPP PA codes ALGEBRACDB (Gilkey, 1996), PANEL (Garner, 2003), SUMMARIZE (Gilkey, 2005), and CCDFGF (Johnson, 1997 and addendum) to establish mean complementary, cumulative distribution functions (CCDFs) for direct brine releases (DBRs) and total releases for the actinide solubilities calculated for the CRA-2004 PABC and at EDTA concentrations of 10 times and 100 times that used for the PABC. We used these PA codes in a manner identical to that used for the PABC.

1.2 Analysis Plan

We carried out this sensitivity study under the analysis plan (AP) for the CRA-2009 PA (Clayton, 2008, Subsection 2.4). However, our sensitivity study deviated from this AP because we used the code Fracture-Matrix Transport (FMT) (Babb and Novak, 1997 and addenda; Wang, 1998) to calculate the effects of EDTA on the speciation and solubilities of actinide elements (Subsections 1.2, 2.1, and 3.1), despite the fact that FMT was not included in this AP along with the codes PANEL (Garner, 2003) and CCDFGF (Johnson, 1997 and addendum) under Task 4h in Section 3, Table 23, column labeled "Description." Furthermore, FMT was not included in Section 4, Table 24, of the AP (Clayton, 2008). In addition, our sensitivity study deviated from the AP (Clayton, 2008) because Brush and Xiong conducted work on this analysis but were not included along with Long in Table 23, column labeled "Responsible Individual(s) in this AP. Finally, this analysis deviated from the work described in the AP (Clayton, 2008) because the AP stated that an EDTA concentration of 1000 times the concentration used for the PABC would be investigated. We did not complete the work for an EDTA concentration of 1000 times the concentration used for the PABC because, after the AP was written, it became apparent that EDTA concentrations of 10 times and 100 times the concentration used for the PABC bounded the values expected in the LANL – CO inventory report for 2007.

1.3 Software

Table 1 provides information on the software used for this analysis. All of this software has been fully qualified according to the requirements of Sandia's WIPP quality assurance (QA) program.

2 CALCULATIONS

This section describes the methods used for our speciation and solubility calculations (Subsection 2.1) and our PA calculations (Subsection 2.2).

2.1 Methods Used for Speciation and Solubility Calculations

We calculated the speciation and solubilities of An(III), An(IV), An(V) for this sensitivity analysis with the same conceptual models, parameters, and code used for the CRA-2004 PABC, except with EDTA concentrations 10 times and 100 times the concentration used for the PABC. Brush and Xiong (2005a) described the methods used to calculate actinide speciation and solubilities for the PABC; Kanney and Leigh (2005) described the methods used for, and Leigh et al. (2005) the results obtained from the PABC.

We calculated the speciation and solubilities of An(III), An(IV), An(V) in Generic Weep Brine (GWB) and Energy Research and Development Administration (WIPP Well) 6 (ERDA-6) in equilibrium with the solids listed below. Snider (2003) verified that GWB is the average composition of intergranular fluids collected from the Salado Formation (Fm.) at the original stratigraphic horizon of the repository and analyzed by Krumhansl et al. (1991). ERDA-6, the average composition of samples collected from that well by Popielak et al. (1983), is typical of fluids from brine reservoirs in the Castile Fm., which underlies the Salado. Both of these brines have been used extensively for laboratory and modeling studies of WIPP near-field chemistry. Table 2 provides the initial compositions of GWB and ERDA-6 and their predicted compositions after equilibration with: (1) halite ($NaCl$) and anhydrite ($CaSO_4$), two of the most abundant minerals in the Salado; (2) the MgO hydration and carbonation products brucite ($Mg(OH)_2$) and hydromagnesite ($Mg_5(CO_3)_4(OH)_2 \cdot 4H_2O$), respectively; and (3) the An(III)-, An(IV)-, and An(V)-bearing solids $Am(OH)_3$; hydrous, amorphous ThO_2; and $KNpO_2CO_3$. In addition to these solids, which we specified in the input files, FMT predicted that: (1) the solids $Mg_2Cl(OH)_3 \cdot 4H_2O$ and whewellite (Ca oxalate hydrate, or $CaC_2O_4 \cdot H_2O$) would precipitate from GWB; and (2) glauberite ($Na_2Ca(SO_4)_2$) and whewellite would precipitate from ERDA-6 if these brines equilibrate with halite, anhydrite, brucite, and hydromagnesite.

Brush and Xiong (2005b) calculated the dissolved concentrations of the organic ligands acetate ($C_2H_3O_2$), citrate ($C_6H_5O_7$), EDTA ($C_{10}H_{16}N_2O_8$), and oxalate (C_2O_4) for the CRA-2004 PABC actinide-solubility calculations. The concentrations of organic ligands calculated by Brush and Xiong (2005b, Table 4, column labeled "PABC") are acetate: 1.06×10^{-2} M; citrate: 8.06×10^{-4} M; EDTA: 8.14×10^{-6} M; and oxalate: 4.55×10^{-2} M. Therefore, we used EDTA concentrations of 8.14×10^{-6}, 8.14×10^{-5}, and 8.14×10^{-4} for this analysis.

Brush and Xiong (2005b) used a mass of 25.6 kg of $H_3NaEDTA$ in the WIPP inventory (Crawford, 2003; Crawford and Leigh, 2003, Leigh, 2005a; Leigh, 2005b) and a brine volume of

10,011 m^3 (Stein, 2005) to calculate the dissolved concentration of EDTA in a homogeneous, 10-panel PA repository. Crawford (2003) reported that all of the EDTA in the WIPP inventory is $H_3NaEDTA$. Crawford and Leigh (2003) and Leigh (2005a) reported that there are 25.6 kg of EDTA in the inventory. Therefore, Leigh (2005b, Table 1, column labeled "Total") corrected Crawford and Leigh (2003) and Leigh (2005a) by stating that there are 25.6 kg of $H_3NaEDTA$ in the inventory. Thus, the EDTA concentrations of 8.14×10^{-6}, 8.14×10^{-5}, and 8.14×10^{-4} M that we used for this analysis correspond to masses of 25.6, 256, and 2560 kg of $H_3NaEDTA$ in the inventory.

We used the geochemical speciation and solubility code FMT, Version 2.4 (Babb and Novak, 1997 and addenda; Wang, 1998), to calculate actinide speciation and solubilities with EDTA concentrations of 10 times and 100 times the concentration used for the CRA-2004 PABC. We did not recalculate these solubilities with the EDTA concentration used for the PABC; instead, we used the solubilities calculated for the PABC by Brush and Xiong (Brush, 2005, Table 5, Runs 7 and 11).

FMT calculates the speciation and solubilities of Am(III), Th(IV), and Np(V) using thermodynamic models based on data obtained using Nd(III), Am(III), and Cm(III); Th(IV); and Np(V). We used the oxidation-state analogy to apply the speciation and solubilities calculated for Am(III) to Pu(III); and for Th(IV) to U(IV), Np(IV), and Pu(IV). We used the speciation and solubilities calculated for Np(V) only for Np(V). This is consistent with the use of the oxidation-state analogy for the WIPP CCA PA (Novak et al., 1996; U.S. DOE, 1996, Appendix SOTERM); the PAVT (Novak, 1997; U.S. EPA, 1998a; 1998b; 1998c) the CRA-2004 PA (U.S. DOE, 2004, Appendix PA, Attachment SOTERM); and the CRA-2004 PABC (Brush and Xiong, 2005a; Brush, 2005).

2.2 Methods Used for PA Calculations

We used the PA codes ALGEBRACDB, PANEL, SUMMARIZE, and CCDFGF to establish mean CCDFs for DBRs and total releases for the actinide solubilities calculated at each of the EDTA concentrations provided in Subsection 2.1 (see above).

We used ALGEBRACDB, Version 2.35 (Gilkey, 1996), to modify the computational data base (CDB) files for PANEL by replacing the solubilites calculated for the CRA-2004 PABC (the "base" solubilities unadjusted by sampled values from the uncertainty ranges established by Xiong et al. (2005) for the PABC) with the new base solubilities calculated with EDTA concentrations of 10 times and 100 times the concentration used for the PABC.

Next, we used PANEL, Version 4.03 (Garner, 2003), to re-establish the actinide source term with the new base solubilities, the actinide oxidation states sampled for the CRA-2004 PABC, and the uncertainty values sampled for the CRA-2004 PABC. PANEL computed the new dissolved (soluble) concentrations; the new colloidal concentrations; and the new total mobilized (dissolved plus colloidal) concentrations. U.S. DOE (2004, Appendix PA, Attachment SOTERM), Brush and Xiong (2005a), Xiong et al. (2005), Brush and Xiong (2005b), Brush (2005), and Garner (2005) provided detailed explanations of how the actinide source term was established for the PABC.

After the PANEL calculations, we used SUMMARIZE, Version 3.01 (Gilkey, 2005), to extract binary data files from the CDBs and write ASCII files for CCDFGF (see below).

Finally, CCDFGF, Version 5.02 (Hansen, 2003), read the new ASCII files and the input files previously generated for the CRA-2004 PABC (all of the other input files) and calculated the mean CCDFs for DBRs and total releases. Helton et al. (1998) explained (1) CCDFs and how they are used to asses compliance with the EPA's containment requirements for the WIPP, (2) DBRs and other releases that contribute to the total releases predicted by WIPP PA, and (3) other aspects of WIPP PA. Vugrin (2005) provided the results of the CCDFGF calculations for the CRA-2004 PABC.

3 RESULTS

This section presents the results of our speciation and solubility calculations (Subsection 3.1), our PA calculations (Subsection 3.3), and the run-control information for this analysis (Subsection 3.4).

3.1 Results of Speciation and Solubility Calculations

Tables 3 and 4 provide the results of our actinide-solubility calculations for the brines GWB and ERDA-6, respectively. These results show that increasing the EDTA concentration to 10 times and 100 times the concentration used for the CRA-2004 PABC increased the solubility of An(III), but not those of An(IV) and An(V).

Inspection of the table entitled “Table of Concentrations for Batch System” in the FMT output files for the CRA-2004 PABC and for this analysis shows that the three predominant An(III) species predicted in GWB with the PABC concentration of EDTA present are: $Am(OH)_2^+$: 2.07×10^{-7} M; $AmEDTA^-$: 1.75×10^{-7} M; and $AmOH^{2+}$: 2.46×10^{-9} M. Increasing the EDTA concentration in GWB to 10 times the PABC concentration increased the predicted concentration of $AmEDTA^-$, but not the concentrations of $Am(OH)_2^+$ and $AmOH^{2+}$; the predominant Am species predicted at this EDTA concentration are: $AmEDTA^-$: 1.75×10^{-6} M; $Am(OH)_2^+$: 2.07×10^{-7} M; and $AmOH^{2+}$: 2.46×10^{-9} M. Similarly, the predominant Am species predicted for an EDTA concentration 100 times that used for the PABC are: $AmEDTA^-$: 1.75×10^{-5} M; $Am(OH)_2^+$: 2.06×10^{-7} M; and $AmOH^{2+}$: 2.47×10^{-9} M. Thus, the increase in the solubility of Am(III) (the sum of all of the dissolved Am(III) species) with increasing EDTA concentration was caused by the high strength of the $AmEDTA^-$ complex relative to those of the $Am(OH)_2^+$ and $AmOH^{2+}$ complexes (Table 5). Note that the solubility-controlling solid predicted by all of these runs with GWB is $Am(OH)_3$.

FMT predicted similar results for ERDA-6. The three predominant Am(III) species predicted in ERDA-6 for the CRA-2004 PABC concentration of EDTA are: $AmEDTA^-$: 1.86×10^{-7} M; $Am(OH)_2^+$: 9.99×10^{-8} M; and $AmOH^{2+}$: 7.04×10^{-10} M. The predominant Am species predicted at an EDTA concentration 10 times that used for the PABC are: $AmEDTA^-$: 1.86×10^{-6} M; $Am(OH)_2^+$: 9.99×10^{-8} M; and $AmOH^{2+}$: 7.04×10^{-10} M. Those predicted for an EDTA concentration 100 times that used for the PABC are: $AmEDTA^-$: 1.86×10^{-5} M; $Am(OH)_2^+$: 9.99×10^{-8} M; and $AmOH^{2+}$: 7.07×10^{-10} M. As with GWB, the increase in the solubility of Am(III) in ERDA-6 with increasing EDTA concentration resulted from the high strength of the $AmEDTA^-$ complex relative to the $Am(OH)_2^+$ and $AmOH^{2+}$ complexes (Table 5). The solubility-controlling solid predicted by all of these runs with ERDA-6 is also $Am(OH)_3$.

In the case of Th(IV), the predominant species predicted by FMT are $Th(OH)_4$(aqueous) and $Th(OH)_3(CO_3)^-$ in both GWB and ERDA-6. The predicted concentrations of these species are about (4-5) $\times 10^{-8}$ M and (1-3) $\times 10^{-8}$ M, respectively, and were unaffected by the EDTA concentration. The concentrations of other species, such as $Th(CO_3)_5^{6-}$, $Th(SO_4)_3^{2-}$, and ThEDTA(aqueous), were always predicted to be 7-11 orders of magnitude lower than those of $Th(OH)_4$(aqueous) and $Th(OH)_3(CO_3)^-$. Although increasing the concentration of EDTA increased the concentration of ThEDTA(aqueous) somewhat, the concentration of this species never increased above 7.42×10^{-15} M, which was not high enough to increase the solubility of Th(IV). This is because the $Th(OH)_4$ and $Th(OH)_3(CO_3)^-$ complexes are much stronger than the ThEDTA complex (Table 5), and prevent EDTA from increasing the concentration of ThEDTA and the solubility of Th(IV). The solubility-controlling solid predicted by all of these runs is hydrous, amorphous ThO_2.

For Np(V), the predominant species predicted by FMT are NpO_2^+, $NpO_2CO_3^-$, and NpO_2Ac in GWB ("Ac" denotes the organic ligand acetate, $CH_3CO_2^-$); and $NpO_2CO_3^-$, NpO_2^+, and NpO_2Ac in ERDA-6. The predicted concentrations of these species varied from about 7×10^{-8} M to 4×10^{-7} M, and were unaffected by the EDTA concentration. The concentration of NpO_2EDTA^{3-}, the strongest Np(V)-EDTA complex, was always predicted to be two-to-six orders of magnitude lower than those of NpO_2^+, $NpO_2CO_3^-$, and NpO_2Ac. Although increasing the concentration of EDTA increased the concentration of NpO_2EDTA^{3-} more than that of ThEDTA(aqueous), the concentration of NpO_2EDTA^{3-} never exceeded 5.45×10^{-10} M, which was not high enough to increase the solubility of Np(V) noticeably. This is because the NpO_2^+, $NpO_2CO_3^-$, and NpO_2Ac complexes are much stronger than NpO_2EDTA^{3-}, and prevent EDTA from increasing the concentration of NpO_2EDTA^{3-} and the solubility of Np(V). The solubility-controlling solid predicted by all of these runs is $KNpO_2CO_3$.

According to the oxidation-state analogy, which has been used for WIPP PA since the 1996 CCA PA (Novak et al., 1996; U.S. DOE, 1996, Appendix SOTERM; Novak, 1997; U.S. EPA, 1998a; 1998b; 1998c; U.S. DOE, 2004, Attachment PA, Appendix SOTERM; Brush and Xiong, 2005a; Brush, 2005), the speciation and solubilities calculated for Am(III) are applicable to Pu(III); and those calculated for Th(IV) are applicable to U(IV), Np(IV), and Pu(IV). The speciation and solubilities calculated for Np(V) apply only to Np(V).

The actinide elements in the TRU waste to be emplaced in the WIPP are, in order of decreasing importance to PA: Pu ~ Am >> U > Th >> Np (Helton et al. 1998). WIPP PA specifies a probability of 0.5 that these elements will speciate in the WIPP as Pu(III), Am(III), U(IV), Th(IV), and Np(IV); and a probability of 0.5 that they will speciate as Pu(IV), Am(III), U(VI), Th(IV), and Np(V) (U.S. DOE, 1996, Appendix SOTERM; U.S. DOE, 2004, Attachment PA, Appendix SOTERM; Brush and Xiong, 2005a; Brush, 2005). The solubilities of actinides in the +III and +IV oxidation states are thus potentially important from the standpoint of the long-term performance of the WIPP, because one or both of the most important actinide elements in the waste (Pu and Am) could occur in these oxidation states. Thus, the conclusion that increasing the EDTA concentration increased the predicted solubility of An(III) (Pu(III) and Am(III)) (see above) is potentially important for WIPP PA, even though increasing the EDTA concentration did not increase the solubility of An(IV) ((Pu(IV), U(IV), Th(IV), and Np(IV)).

On the other hand, the +V actinide oxidation state is the least important of the four oxidation states in which actinide elements could speciate in the WIPP. This is because: (1) Np is the only one of the actinides listed above expected to speciate in the +V oxidation state, and (2) Np is not important from the standpoint of WIPP PA. In fact, release of all of the Np in the WIPP inventory would have no effect on the long-term performance of the WIPP (Brush and Garner, 2005).

We did not include An(VI) in the sensitivity calculations described above because a thermodynamic speciation and solubility model has not been developed for An(VI). The +VI actinide oxidation state is more important than An(V) but not as important as An(III) and An(IV), because: (1) U is the only actinide listed above expected to speciate as An(VI), and (2) U is much less important than Pu or Am. Although we could not include U(VI) in our sensitivity calculations, Wall and Wall (2004) demonstrated that organic ligands would have a very limited effect on the solubility of U(VI).

3.2 Effects of Transition Metals and Na on the Solubility of Pu(III) and Am(III)

It is important to point out that our An(III), An(IV), and An(V) speciation and solubility models do not include several metals that will be or could be present in large quantities in the repository, that will dissolve in brines to at least some extent, and that will form strong complexes with EDTA. These include: (1) Mn, which reacts with dissolved EDTA to form the complex $MnEDTA^{2-}$ ($\log Q_{I = 0.1\ M} = 13.89$); (2) Fe, which forms $FeEDTA^{2-}$ ($\log Q_{I = 0.1\ M} = 14.30$); (3) Co, which forms $CoEDTA^{2-}$ ($\log Q_{I = 0.1\ M} = 16.45$); (4) Ni, which forms $NiEDTA^{2-}$ ($\log Q_{I = 0.1\ M} = 18.4$); (5) Zn, which forms $ZnEDTA^{2-}$ ($\log \beta_{I = 0\ M} = 18.0$); and (6) Pb, which forms $PbEDTA^{2-}$ ($\log Q_{I = 0.1\ M} = 18.0$). The values of β (the thermodynamic stability constant or Q (the solubility quotient) for these complexes are from Smith et al. (2004) unless otherwise noted, and pertain to the ionic strength (I) given for each complex. However, it is likely that metals that form strong complexes with EDTA at $I = 0$ or 0.1 would also form strong complexes with this organic ligand at 7.66 or 6.80 m, the ionic strengths predicted for GWB and ERDA-6, respectively, after equilibration with brucite, hydromagnesite, halite, anhydrite, and other solids (see Table 2).

Metallic Fe or Pb and/or their corrosion products will certainly be present in large quantities in the repository, and will compete very effectively for EDTA with Pu(III) and Am(III). This is especially true in the case of Pb, for which $\log Q_{I = 0.1\ M} = 18.0$ – a value nearly equal to $\log \beta$ for $AmEDTA^-$ (18.9699). This will in turn decrease the extent to which EDTA will increase the solubility of Pu(III) and Am(III). In other words, the effect of EDTA on the solubility of Pu(III) and Am(III) predicted by our An(III) solubility model (Tables 3 and 4) is conservative. However, we cannot include the effects of Fe and Pb in our models because we do not have enough Pitzer ion-interaction parameters for dissolved Fe and Pb species yet. (Development of Pitzer parameters for Fe and Pb is underway so that the effects of these elements can be included in future calculations.) Furthermore, Fe and Pb will not eliminate the effects of EDTA on the solubility of Pu(III) and Am(III) because formation of sulfides such as mackinawite ($Fe_{1-x}S$) and galena (PbS) in the repository will limit the solubilities of Fe and Pb.

Furthermore, Mn, Co, Ni, and Zn also could be present in the repository in large quantities, especially as constituents of steels in the waste. If so, these elements would dissolve as the steels corrode, and could also decrease the extent to which EDTA will increase the solubility of Pu(III) and Am(III).

Finally, Na in WIPP brines will react with EDTA to form the complex $NaEDTA^{3-}$. This complex is weak relative to $AmEDTA^{-}$. Smith et al (2004) provided log $Q_{I = 0.1 \text{ M}} = 1.86$, and Xia et al. (2003) obtained an $I = 0$ value (log β) of 2.7. However, the concentration of Na is very high in WIPP brines (see Table 2), so the high concentration of Na will make up for the weakness of the $NaEDTA^{3-}$ complex to some extent. Thus, Na could also decrease the extent to which EDTA will increase the solubility of Pu(III) and Am(III).

3.3 Results of PA Calculations

Figures 1 and 2 show the effects on DBRs and total releases, respectively, of dissolved EDTA concentrations 1 times, 10 times, and 100 times the concentration used for the CRA-2004 PABC solubility calculations.

Figure 1 shows that increasing the EDTA concentration to 10 times and 100 times the concentration used for the PABC solubilities affects DBRs. The effect is noticeable at all probabilities in Figure 1, but becomes more noticeable at probabilities between 0.01 and 0.1.

Figure 2 shows that increasing the EDTA concentration to 10 times and 100 times the concentration used for the PABC solubilities also affects total releases. The effect of EDTA on total releases becomes noticeable at probabilities between 0.1 and 1, and becomes more noticeable at probabilities between 0.01 and 0.1; this is because DBRs become the dominant release mechanism at probabilities between 0.01 and 0.1. (Cuttings and cavings releases are the dominant release mechanism at higher probabilities.)

However, Figures 1 and 2 show that the WIPP would still comply with the release limits specified in Section 191.13 of the EPA's containment requirements (U.S. EPA, 1985; 1993) even if the EDTA concentration were 100 times the concentration used for the PABC solubilities. (Brush and Xiong (2005b) used a mass of 25.6 kg of $H_3NaEDTA$ in the WIPP inventory (Crawford, 2003, Crawford and Leigh, 2003; Leigh, 2003; Leigh, 2005a; Leigh, 2005b) to calculate the EDTA concentration of 8.14×10^{-6} M that was used for the actinide solubility calculations for the PABC; therefore, an EDTA concentration 100 times the PABC concentration corresponds to 2560 kg of $H_3NaEDTA$ in the inventory.

3.4 Run-Control Information

Table 6 provides the run-control information for the FMT calculations carried out for this analysis. Tables 7, 8 and 9 provide the run-control information for the PANEL calculations conducted for this analysis; Tables 10, 11, and 12 provide this information for the CCDFGF calculations.

4 CONCLUSIONS

Increasing the concentration of EDTA in WIPP brines from its PABC concentration of 8.14×10^{-6} M to values 10 times and 100 times the PABC concentration increased the solubility of An(III) in both GWB and ERDA-6, but not those of An(IV) and An(V) (Tables 3 and 4).

Increasing the EDTA concentration to 10 times and 100 times the PABC concentration affected DBRs and total releases, especially at low probabilities (Figures 1 and 2). However, the WIPP would still comply with the EPA's containment requirements (U.S. EPA, 1985; 1993) even if the EDTA concentration were 100 times the PABC concentration.

Our An(III), An(IV), and An(V) speciation and solubility models do not include several metals that will be or could be present in large quantities in the repository, that will dissolve in brines to at least some extent, and that form strong complexes with EDTA (Subsection 3.2). These include Mn, Fe, Co, Zn, and Pb. Metallic Fe or Pb and/or their corrosion products will certainly be present in large quantities in the WIPP and will compete very effectively with Pu(III) and Am(III) for EDTA. This will in turn decrease the extent to which EDTA will increase the solubility of Pu(III) and Am. In other words, the effect of EDTA on the solubility of Pu(III) and Am(III) predicted by our An(III) solubility model (Tables 3 and 4) is very conservative. However, we cannot include the effects of Fe and Pb in our models because we do not have enough Pitzer ion-interaction parameters for dissolved Fe and Pb species yet. (Development of Pitzer parameters for Fe and Pb is underway so that the effects of these elements can be included in future calculations.)

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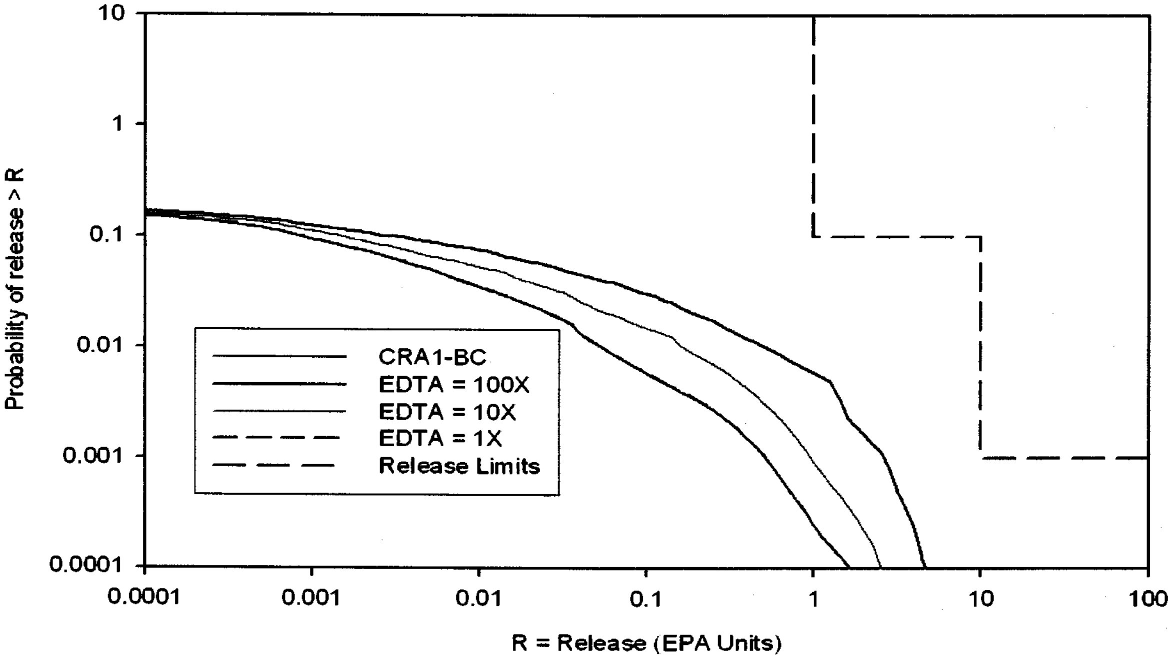

Figure 1. Effects of EDTA concentrations 1 times, 10 times, and 100 times the concentration used for the CRA-2004 PABC on the mean CCDF for DBRs. Please note that our recalculation of the mean CCDF for DBRs using the solubilities calculated for the PABC by Brush and Xiong (Brush, 2005, Table 5, Runs 7 and 11) (EDTA = 1× in the legend box) is indistinguishable from the mean CCDF for DBRs from the PABC (CRA1-BC in the legend box).

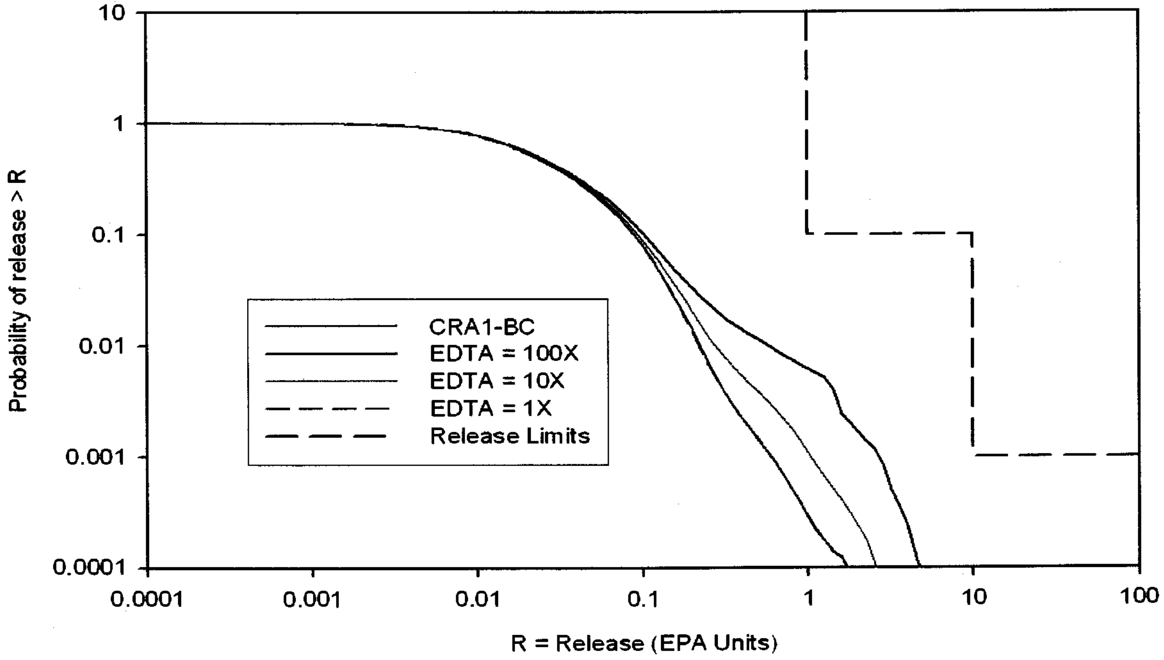

Figure 2. Effects of EDTA concentrations 1 times, 10 times, and 100 times the concentration used for the CRA-2004 PABC on the mean CCDF for total releases. Please note that our recalculation of the mean CCDF for total releases using the solubilities calculated for the PABC by Brush and Xiong (Brush, 2005, Table 5, Runs 7 and 11) (EDTA = 1× in the legend box) is indistinguishable from the mean CCDF for total releases from the PABC (CRA1-BC in the legend box).

Table 1. Software Used for This Analysis.

Code	Version	Executable	Build Date	CMS Library	CMS Class
ALGEBRACDB	2.35	ALGEBRACDB_PA96.EXE	31-01-96	LIBALG	PA96
CCDFGF	5.02	CCDFGF_QB0502.EXE	13-12-04	LIBCCGF	QB0502
FMT	2.4	FMT_QB0204.EXE	03-09-98	LIBFMT	QB0204
PANEL	4.03	PANEL_QA0403.EXE	25-04-05	LIBPANEL	QA0403
PRECCDFGF	1.01	PRECCDFGF_QA0101.EXE	07-07-05	LIBCCGF	QA0101
SUMMARIZE	3.01	SUMMARIZE_QB0301.EXE	21-12-05	LIBSUM	QB0301

Table 2. Compositions of GWB and ERDA-6 (M, Unless Otherwise Noted) Before and After Equilibration with Brucite, Hydromagnesite, Halite, Anhydrite, and Other Solids (see Subsection 2.1).

Element or Property	GWB Before Reaction with Solids[A]	GWB After Reaction with Solids[B]	ERDA-6 Before Reaction with Solids[C]	ERDA-6 After Reaction with Solids[D]
$B(OH)_x^{3-x}$	0.158	0.166	0.063	0.0624
Na^+	3.53	4.35	4.87	5.24
Mg^{2+}	1.02	0.578	0.019	0.157
K^+	0.467	0.490	0.097	0.0961
Ca^{2+}	0.014	0.00895	0.012	0.0107
SO_4^{2-}	0.177	0.228	0.170	0.179
Cl^-	5.86	5.38	4.8	5.24
Br^-	0.0266	0.0278	0.011	0.0109
Total inorganic C	-	0.350 mM	16 mM	0.428 mM
Ionic strength	-	7.66 m	-	6.80 m
$\log f_{CO_2}$	-	-5.50	-	-5.50
pH	-	8.69	6.17	8.94
Relative humidity	-	0.732	-	0.748
Specific gravity	1.2	1.23	1.216	1.22

A. From Krumhansl et al. (1991) and Snider (2003).
B. FMT Run 7 (Brush, 2005).
C. From Popielak et al. (1993).
D. FMT Run 11 (Brush, 2005).

Table 3. Actinide Solubilities in GWB (M) Predicted by FMT.

Actinide Ox. State	EDTA = PABC Conc.	EDTA = 10 × PABC Conc.	EDTA = 100 × PABC Conc.
+III	3.87×10^{-7}	1.96×10^{-6}	1.77×10^{-5}
+IV	5.64×10^{-8}	5.64×10^{-8}	5.64×10^{-8}
+V	3.55×10^{-7}	3.54×10^{-7}	3.54×10^{-7}

Table 4. Actinide Solubilities in ERDA-6 (M) Predicted by FMT.

Actinide Ox. State	EDTA = PABC Conc.	EDTA = 10 × PABC Conc.	EDTA = 100 × PABC Conc.
+III	2.88×10^{-7}	1.96×10^{-6}	1.87×10^{-5}
+IV	6.79×10^{-8}	6.79×10^{-8}	6.79×10^{-8}
+V	8.24×10^{-7}	8.24×10^{-7}	8.25×10^{-7}

Table 5. Logarithms of the Stability Constants of the Dominant Am(III), Th(IV) and Np(V) Aqueous Species in the FMT Database (Xiong, 2005).

Am(III) Species	Log β (Am(III) Species)	Th(IV) Species	Log β (Th(IV) Species)	Np(V) Species	Log β (Np(V) Species)
$AmEDTA^-$	18.9699	$Th(OH)_4(aq)$	38.4862	NpO_2^+	See A.
$Am(OH)_2^+$	12.3017	$Th(OH)_3(CO_3)^-$	38.2832	$NpO_2CO_3^-$	5.0169
$AmOH^{2+}$	6.4410	$ThEDTA(aq)$	23.5568	NpO_2Ac	1.3737
-	-	-	-	NpO_2EDTA^{3-}	8.5351

A. There is no stability constant for NpO_2^+ because this species is formed by the dissolution of $KNpO_2CO_3$, the solubility-controlling solid for Np, via the dissolution-precipitation reaction: $KNpO_2CO_3 \rightleftharpoons K^+ + NpO_2^+ + CO_3^{2-}$.

Table 6. Run-Control Information for the FMT Calculations Carried Out for This Analysis.

	File Names[1,2,3]	CMS Library	CMS Class
Script:			
Script	EVAL_FMT.COM	LIBEDTA_EVAL	EDTA-0
Script Input	EVAL_FMT_EDTA_*w*_HMAG_ORGS_*a*.INP	LIBEDTA_EVAL	EDTA-0
Script Log	EVAL_FMT_EDTA_*w*_HMAG_ORGS_*a*.LOG	LIBEDTA_FMT	EDTA-0
FMT:			
Input	FMT_050405.CHEMDAT	LIBEDTA_FMT	EDTA-0
Input	FMT_GENERIC.RHOMIN	LIBEDTA_FMT	EDTA-0
Input	FMT_EDTA_*w*_HMAG_ORGS_*a*_*n*.IN	LIBEDTA_FMT	EDTA-0
Input	FMT_EDTA_*w*_HMAG_ORGS_*a*_*n*.INGUESS	LIBEDTA_FMT	EDTA-0
Output	FMT_EDTA_*w*_HMAG_ORGS_*a*_*n*.OUT	LIBEDTA_FMT	EDTA-0
Output	FMT_EDTA_*w*_HMAG_ORGS_*a*_*n*.FOR088	Not kept	Not kept

---

1. $w \in \{\text{ER6, GWB}\}$.
2. $a \in \{\text{C, X}\}$ for each W. X = 10 times the PABC EDTA concentration; C = 100 times the PABC EDTA concentration.
3. $n \in \{\text{007 for each GWB, 011 for each ER6}\}$.

Table 7. PANEL Run-Control Scripts.

Step	Codes Run in Step	Scripts	CMS Library	CMS Class
3	ALGEBRACDB	EVAL_PANEL_STEP3_EDTA.COM	LIBEDTA_EVAL	EDTA-0
4	PANEL	EVAL_PANEL_STEP4.COM	LIBEDTA_EVAL	EDTA-0

Table 8. PANEL Step 3 Input and Output Files.

	File Names[1,2]	CMS Library	CMS Class
Script:			
Script Input	EVAL_PANEL_EDTA*x*X_STEP3_R1.INP	LIBEDTA_EVAL	EDTA-0
Script Log	EVAL_PANEL_EDTA*x*X_STEP3_R1.LOG	LIBEDTA_PANEL	EDTA-0
ALGEBRACDB			
Input	ALG_PANEL_EDTA*x*X.INP	LIBEDTA_PANEL	EDTA-0
Input	LHS3_PANEL_CRA1BC_R1_V*vvv*.CDB	LIBCRA1BC_PANEL	EDTA-0
Output	ALG_PANEL_EDTA*x*X_R1_V*vvv*.CDB	LIBEDTA_PANEL	EDTA-0
Output	ALG_PANEL_EDTA*x*X_R1_V*vvv*.DBG	Not kept	Not kept

---

[1] $x \in \{1, 10, 100\}$.

[2] $vvv \in \{001, 002, ..., 100\}$ for each intrusion time .

Table 9. PANEL_CON (Concentration) Step 4 Input and Output Files.

	File Names[1,2,3]	CMS Library	CMS Class
Script:			
Script Input	EVAL_PANEL_EDTA*x*X_STEP4_R1.INP	LIBEDTA_EVAL	EDTA-0
Script Log	EVAL_PANEL_EDTA*x*X_STEP4_R1.LOG	LIBEDTA_PANEL	EDTA-0
PANEL_CON:			
Input	ALG_PANEL_EDTA*x*X_R1_V*vvv*.CDB	LIBEDTA_PANEL	EDTA-0
Output	PANEL_CON_EDTA*x*X_R1_S*s*_*Vvvv*.CDB	LIBEDTA_PANEL	EDTA-0
Output	PANEL_CON_EDTA*x*X_R1_S*s*_*Vvvv*.DBG	Not kept	Not kept

---

1. $x \in \{1, 10, 100\}$.
2. $s \in \{1, 2, 3, 4, 5\}$.
3. $vvv \in \{001, 002, ..., 100\}$ for each s.

Table 10. CCDF Input Tabulation Run-Control Scripts.

Code	Script	Script CMS Library	Script CMS Class
SUMMARIZE	EVAL_SUM.COM SUB_SUM.COM	LIBEDTA_EVAL	EDTA-0

Table 11. CCDF Input Tabulation Input and Output Files.

	File Names[1,2,3]	CMS Library	CMS Class
Script:			
Input	EVAL_SUM_PANEL_CON_EDTA*x*X_R1_S*s*.INP	LIBEDTA_EVAL	EDTA-0
Input	SUM_PANEL_CON_CRA1BC.TMPL	LIBCRA1BC_SUM	EDTA-0
Output	SUM_PANEL_CON_EDTA*x*X_R1_S*s*.INP	LIBEDTA_SUM	EDTA-0
Log	EVAL_SUM_PANEL_CON_EDTA*x*X_R1_S*s*.LOG	LIBEDTA_SUM	EDTA-0
SUMMARIZE:			
Input	SUM_PANEL_CON_EDTA*x*X_R1_S*s*.INP	LIBEDTA_SUM	EDTA-0
Input	PANEL_CON_EDTA*x*X_R1_S*s*_*Vvvv*.CDB	LIBEDTA_PANEL	EDTA-0
Output	SUM_PANEL_CON_EDTA*x*X_R1_S*s*.TBL	LIBEDTA_SUM	EDTA-0
Output	SUM_PANEL_CON_EDTA*x*X_R1_S*s*.DBG	Not kept	Not kept

---

1. $x \in \{1, 10, 100\}$.
2. $s \in \{1, 2\}$.
3. $vvv \in \{001, 002, ..., 100\}$.

Table 12. CCDF Construction Step 3 Input and Output Files.

	File Names[1-7]	CMS Library	CMS Class
Script:			
Script	EVAL_CCGF_STEP3.COM	LIBEDTA_EVAL	EDTA-0
Script	SUB_CCGF_STEP3.COM	LIBEDTA_EVAL	EDTA-0
Script Input	EVAL_CCGF_STEP3_EDTA*x*X_R1.INP	LIBEDTA_EVAL	EDTA-0
Script Log	EVAL_CCGF_STEP3_EDTA*x*X_R1.LOG	LIBEDTA_CCGF	EDTA-0
PRECCDFGF:			
Input	INTRUSIONTIMES.IN	LIBCRA1BC_CCGF	EDTA-0
Input	MS_CCGF_CRA1BC.CDB	LIBCRA1BC_CCGF	CRA1BC-1
Input	LHS3_CCGF_CRA1BC_R1_V*vvv*.CDB	LIBCRA1BC_CCGF	CRA1BC-1
Input	SUM_DBR_CRA1BC_R1_S*s*_T*tttt*_*c*.TBL	LIBCRA1BC_SUM	CRA1BC-1
Input	CUSP_CRA1BC_R1.TBL	LIBCRA1BC_CUSP	CRA1BC-0
Input	SUM_NUT_CRA1BC_R1_S1.TBL	LIBCRA1BC_SUM	CRA1BC-1
Input	SUM_NUT_CRA1BC_R1_S*s*_T*tttt*.TBL	LIBCRA1BC_SUM	CRA1BC-1
Input	SUM_PANEL_INT_CRA1BC_R1_S6_T*tttt*.TBL	LIBCRA1BC_SUM	CRA1BC-0
Input	SUM_ST2D_CRA1BC_R1_M*m*.TBL	LIBCRA1BC_SUM	CRA1BC-0
Input	EPU_CRA1BC_*h*H.DAT	LIBCRA1BC_EPU	CRA1BC-2
Input	SUM_PANEL_CON_EDTA*x*X_R1_S*s*.TBL	LIBEDTA_SUM	EDTA-0
Input	SUM_PANEL_ST_CRA1BC_R1_S*s*.TBL	LIBCRA1BC_SUM	CRA1BC-0
Output	CCGF_EDTA*x*X_RELTAB_R1.DAT	LIBEDTA_CCGF	EDTA-0

(Table 12 continued on next page)

Table 12. CCDF Construction Step 3 Input and Output Files (continued).

	File Names$^{1\text{-}7}$	CMS Library	CMS Class
CCDFGF:			
Input	CCGF_CRA1BC_CONTROL_R1.INP	LIBCRA1BC_CCGF	EDTA-0
Input	CCGF_EDTA*x*X_RELTAB_R1.DAT	LIBEDTA_CCGF	EDTA-0
Output	CCGF_EDTA*x*X_R1.OUT	LIBEDTA_CCGF	EDTA-0
Output	CCGF_EDTA*x*X_R1.DBG	Not kept	Not kept

---

[1] $x \in \{1, 10, 100\}$.

[2] $vvv \in \{001, 002, ..., 100\}$ for each r.

[3] $s \in \begin{cases} \{1, 2, 3, 4, 5\} \text{ for SUM\_DBR} \\ \{2, 3, 4, 5\} \text{ for SUM\_NUT} \\ \{1, 2\} \text{ for SUM\_PANEL\_CON and SUM\_PANEL\_ST} \end{cases}.$

[4] $ttttt \in \begin{cases} \{00100, 00350, 01000, 03000, 05000, 10000\} \text{ for S1 for each } r \text{ for SUM\_DBR} \\ \{00550, 07500, 02000, 04000, 10000\} \text{ for S2, S4 for each } r \text{ for SUM\_DBR} \\ \{\ 01200, 01400, 03000, 05000, 10000\} \text{ for S3, S5 for each } r \text{ for SUM\_DBR} \\ \{00100, 00350\} \text{ for S2, S4 for each } r \text{ for SUM\_NUT} \\ \{01000, 03000, 05000, 07000, 09000\} \text{ for S3, S5 each } r \text{ for SUM\_NUT} \\ \{00100, 00350, 01000, 02000, 04000, 06000, 09000\} \text{ for each } r \text{ for SUM\_PANEL\_INT} \end{cases}.$

[5] $c \in \{\text{L, M, U}\}$for each intrusion for SUM_DBR .

[6] $m \in \{\text{F, P}\}$.

[7] $h \in \{\text{C, H}\}$.

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