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Sandia National Laboratories
Waste Isolation Pilot Plant

Predictions of the Compositions of Standard WIPP Brines as a Function of pCH for Laboratory Studies of the Speciation and Solubilities of Actinides

Work Carried Out under Task 1 of the Analysis Plan for WIPP Near-Field
Geochemical Process Modeling, AP 153, Rev. 0.
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1 INTRODUCTION

This analysis report provides the results of our predictions of the compositions of the standard Waste Isolation Pilot Plant (WIPP) brines Generic Weep Brine (GWB) and Energy Research and Development Administration (WIPP Well) 6 (ERDA-6) during and after reactions with the solids in WIPP disposal rooms and other reactants. 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.

These predictions provide compositions of GWB and ERDA-6 intermediate between their in situ compositions and those expected after equilibration with solids and other reactants. We will provide these compositions to Los Alamos National Laboratory — Carlsbad Operations (LANL — CO) so that LANL — CO personnel can use them to synthesize brines for experiments to determine the effects of the pH on the speciation and solubilities of actinide elements in the repository (e.g., Lucchini et al., 2007; Borkowski et al., 2009; Borkowski, 2010).

We used EQ3/6, Version 8.0a (Wolery and Jarek, 2003; Wolery, 2008; Wolery et al., 2010) for this analysis. Wolery et al. (2010) completed the qualification of this version of EQ3/6 according to Sandia National Laboratories' (SNL's) WIPP QA procedures for WIPP compliance-related actinide solubility calculations.

This analysis was carried out under Task 1 of AP-153 (Brush and Xiong, 2011).

Table 1 (see next page) defines the abbreviations, acronyms, and initialisms used in this report.

Table 1. Abbreviations, Acronyms, and Initialisms.

| Abbreviation, Acronym, or Initialism | Definition |
|--------------------------------------|---|
| A_ϕ | the Debye-Hückel slope of the osmotic coefficient |
| acetate | CH_3COO^- or CH_3CO_2^- |
| Am, Am(III) | americium, americium in the +III oxidation state |
| am | amorphous |
| anhydrite | CaSO_4 |
| AP | analysis plan |
| aq | aqueous |
| aragonite | CaCO_3 , a polymorph of CaCO_3 that is metastable with respect to calcite |
| atm | atmosphere(s) |
| B, B(II) | boron, boron in the +II oxidation state |
| Br, Br(-I) | bromine, bromine in the -I oxidation state |
| brucite | $\text{Mg}(\text{OH})_2$ |
| C | carbon |
| Ca, Ca(II) | calcium, calcium in the +II oxidation state |
| calcite | CaCO_3 , the thermodynamically stable polymorph of CaCO_3 |
| citrate | $(\text{CH}_2\text{COO})_2\text{C}(\text{OH})(\text{COO})^{3-}$ or $(\text{CH}_2\text{CO}_2)_2\text{C}(\text{OH})(\text{CO}_2)^{3-}$ |
| Cl, Cl(-I), Cl^- | chlorine, chlorine in the -I oxidation state, chloride ion |
| CMS | (Sandia/WIPP software) Configuration Management System |
| CO_2 | carbon dioxide |
| CO_3 | carbonate |
| CPR | cellulosic, plastic, and rubber (materials) |
| CRA-2009 | the second WIPP Compliance Recertification Application, submitted to the EPA in March 2009 |
| DB | (thermodynamic) database |
| DOE | (U.S.) Department of Energy |
| dolomite | $\text{CaMg}(\text{CO}_3)_2$, a carbonate mineral that is nucleates and grows slowly under low-temperature conditions and is often suppressed (prevented from forming) in geochemical modeling calculations |
| DRZ | disturbed rock zone |
| EDTA | ethylenediaminetetraacetate, $(\text{CH}_2\text{COO})_2\text{N}(\text{CH}_2)_2\text{N}(\text{CH}_2\text{COO})_2^{4-}$ or $(\text{CH}_2\text{CO}_2)_2\text{N}(\text{CH}_2)_2\text{N}(\text{CH}_2\text{CO}_2)^{4-}$ |
| EPA | (U.S.) Environmental Protection Agency |

Table 1 continued on next page

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

| Abbreviation, Acronym, or Initialism | Definition |
|--|--|
| EQ3/6 | a geochemical software package for speciation and solubility calculations (EQ3NR) and reaction-path calculations (EQ6) |
| ERDA-6 | Energy Research and Development Administration (WIPP Well) 6, a synthetic brine representative of fluids in Castile brine reservoirs |
| f _{CO₂} | fugacity (similar to the partial pressure) of CO ₂ |
| Fm. | Formation |
| g | gaseous |
| GWB | Generic Weep Brine, a synthetic brine representative of intergranular Salado brines at or near the stratigraphic horizon of the repository |
| gypsum | CaSO ₄ ·2H ₂ O |
| H or H ₂ , H ⁺ | hydrogen or hydrogen ion |
| halite | NaCl |
| H ₂ O | water (aq, g, or contained in solid phases) |
| hydromagnesite | Mg ₅ (CO ₃) ₄ (OH) ₂ ·4H ₂ O or Mg ₄ (CO ₃) ₃ (OH) ₂ ·3H ₂ O |
| I | ionic strength |
| K, K(I) | potassium, potassium in the +I oxidation state |
| kg | kilogram(s) |
| LANL — CO | Los Alamos National Laboratory - Carlsbad Operations |
| M | molar |
| m | meter(s) or molal |
| magnesite | MgCO ₃ |
| Mg, Mg(II) | magnesium, magnesium in the +II oxidation state |
| MgO | magnesium oxide, used to refer to the WIPP engineered barrier, which includes periclase as the primary constituent and various impurities |
| mM | millimolar |
| Na, Na(I) | sodium, sodium in the +I oxidation state |
| NBS | (U.S.) National Bureau of Standards |
| Nd, Nd(III) | neodymium, neodymium in the +III oxidation state |
| nesquehonite | MgCO ₃ ·3H ₂ O |
| Np, Np(V) | neptunium, neptunium in the +V oxidation state |
| O or O ₂ | oxygen |

Table 1 continued on next page

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

| Abbreviation, Acronym, or Initialism | Definition |
|--|--|
| OH, OH ⁻ oxalate | hydroxide or hydroxide ion (COO) ²⁻ or C ₂ O ₄ ²⁻ |
| PA | performance assessment |
| PABC | Performance Assessment Baseline Calculations |
| periclase | pure, crystalline MgO, the primary constituent of the WIPP engineered barrier |
| pH | the negative, common logarithm of the activity of H ⁺ |
| pCH | the negative, common logarithm of the molar concentration of H ⁺ |
| phase 3 | Mg ₂ Cl(OH) ₃ ·4H ₂ O |
| phase 5 | Mg ₃ (OH) ₅ Cl·4H ₂ O |
| polyhalite | K ₂ MgCa ₂ (SO ₄) ₄ ·2H ₂ O |
| QA | quality assurance |
| Rev. | revision |
| RH | relative humidity |
| S, S(VI), SO ₄ ²⁻ | sulfur, sulfur in the +VI oxidation state, sulfate ion |
| s | solid |
| SCA | S. Cohen and Associates |
| SNL | Sandia National Laboratories |
| Th, Th(IV) | thorium, thorium in the +IV oxidation state |
| TIC | total inorganic C |
| WIPP | (U.S. DOE) Waste Isolation Pilot Plant |
| wt % | weight percent |
| μ ⁰ /RT | dimensionless standard chemical potential |
| ξ | the EQ6 reaction- progress variable |

2 METHODS

The objective of this analysis was to predict the compositions of the standard WIPP brines GWB (Krumhansl et al., 1991; Snider, 2003) and ERDA-6 (Popielak et al., 1983) during and after reactions with the solids in WIPP disposal rooms and other reactants so that LANL — CO personnel can use them to synthesize brines for experiments to determine the effects of pH on the speciation and solubilities of actinide elements in the repository (e.g., Lucchini et al., 2007; Borkowski et al., 2009; Borkowski, 2010).

We used the geochemical software package EQ3/6, Version 8.0a (Wolery and Jarek, 2003; Wolery, 2008; Wolery et al., 2010) to simulate two reactions for this analysis.

In the first reaction (referred to herein as “run 1”), we added the organic ligands acetate (CH_3COO^-), citrate ($((\text{CH}_2\text{COO})_2\text{C}(\text{OH})(\text{COO})^3^-)$), EDTA (ethylenediaminetetraacetate, $(\text{CH}_2\text{COO})_2\text{N}(\text{CH}_2)_2\text{N}(\text{CH}_2\text{COO})_2^4-$), and oxalate ($((\text{COO})^2^-)$) to GWB and ERDA-6. We then reacted these brines with the important solids in WIPP disposal rooms (see below) in a manner consistent with the conceptual models for WIPP near-field chemistry (SCA, 2008; Brush and Xiong, 2011) to simulate the chemical changes that occur as they evolve from their initial (in situ) compositions to new compositions after equilibration with the solids. After equilibration, the compositions of these brines define so-called invariant points (one each for GWB and ERDA-6), because the solids specified in the conceptual models — especially brucite and hydromagnesite — control the new compositions of the brines and parameters such as the fugacity (similar to the partial pressure) of CO_2 (f_{CO_2}), pH, and total inorganic carbon (TIC).

In the first step of run 1 (step 1), we used the speciation and solubility code EQ3NR to add the organic ligands acetate, citrate, EDTA, and oxalate to GWB and ERDA-6. We set the initial concentrations of acetate, citrate, EDTA, and oxalate equal to those calculated by Brush and Xiong (2009) for the Performance Assessment Baseline Calculation for the second WIPP Compliance Recertification Application (CRA-2009 PABC). We set the initial value of the total inorganic carbon (TIC) concentrations of both brines at 16 mM for this step because: (1) Popielak et al. (1983) reported that the average TIC content of ERDA-6 was 16 mM, (2) the initial TIC of GWB was not determined, so (3) we assumed that the initial TIC content of GWB was equal to that of ERDA-6. (The initial value of the TIC did not affect the values of the TIC predicted during the rest of the calculations). The code charge balanced on H^+ , calculated the f_{CO_2} and pH, speciated all of the dissolved elements and calculated the values of parameters such as f_{CO_2} and TIC, and wrote a “pickup” file (*.3p file) for run 1, step 2. The *.3p file is called a pickup file because it is copied and pasted into an EQ6 input file, and provides all of the information on the solution and solids required for an EQ6 run.

In run 1, step 2, we used the reaction-path code EQ6 to titrate the solids halite (NaCl), anhydrite (CaSO_4), brucite ($\text{Mg}(\text{OH})_2$), $\text{ThO}_2(\text{am})$, KNpO_2CO_3 , and $\text{Am}(\text{OH})_3(\text{s})$ into GWB and ERDA-6. We used halite and anhydrite to simulate the most important minerals in

the Salado Fm. at or near the stratigraphic horizon of the repository; brucite to simulate one of the expected hydration products of MgO (the WIPP engineered barrier); and ThO₂(am), KNpO₂CO₃, and Am(OH)₃(s) to simulate the presence of the solids most likely to control the solubilities of Th(IV), Am(III), and Np(V) in the repository. We had planned to titrate in both brucite and hydromagnesite (Mg₅(CO₃)₄(OH)₂·4H₂O) during this step, but — when we titrated in hydromagnesite — the code did not converge; and the 16 mM TIC concentration that we specified at the start of run 1, step 1, was sufficient to produce enough hydromagnesite for run 1, step 2. As EQ6 titrated in these solids, some of them dissolved and/or others precipitated. EQ6 calculated the moles of solids that dissolved and/or precipitated, speciated all of the dissolved elements; and recalculated the values of parameters such as f_{CO₂}, pCH, TIC, etc. At the end of each run, EQ6 wrote another pickup file (.6p file), which provided all of the information on the solution and solids required for another EQ6 run (see below).

For run 1, step 2, we used quantities of brine, halite, anhydrite, brucite, and hydromagnesite similar to those that will be present in the repository after it is filled and sealed, but scaled down by the same factor used to scale down the quantity of water contained in 17,400 m³ of brine (Clayton, 2008) to 1 kg of water. Clayton (2008) determined that 17,400 m³ of brine is the minimum volume of brine in the repository required for a direct brine release (DBR) from the 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.). EQ3/6 allows the user to specify the composition and specific gravity of the aqueous phase present at the start of a run. However, the code assumes that exactly 1 kg of H₂O is present in the solution and uses the specific gravity entered by the user to calculate the volume of solution. We used spreadsheet calculations to scale down (1) the quantities of halite and anhydrite in the disturbed rock zone (DRZ) surrounding the repository, and (2) the quantity of MgO that will be emplaced in the repository. (The spreadsheet, entitled “AP-153_Tasks 1 and 2, Scaling of Solids.xls,” is in the file AP153Task1Data.zip in library LIBEQ36, class AP153, in the Sandia/WIPP software Configuration Management System, or CMS.) To calculate the quantities of halite and anhydrite, we used the conservatively large DRZ currently implemented in WIPP PA and the assumption that the DRZ comprises 90 wt % halite and 10 wt % anhydrite. This mineralogical composition is similar to Brush’s (1990) interpretation of the results of Stein’s (1985) mineralogical analysis of the Salado Fm. at or near the stratigraphic horizon of the repository: Brush (1990) concluded that, for use in geochemical modeling, the Salado consists of 93.2 wt % halite and 1.7 wt % each of anhydrite, gypsum (CaSO₄·2H₂O), magnesite (MgCO₃), and polyhalite (K₂MgCa₂(SO₄)₄·2H₂O). However, we assumed for this analysis that the Salado contains 90 wt % halite and 10 wt % anhydrite because the conceptual models for WIPP near-field chemistry include only halite and anhydrite (SCA, 2008). For run 1, we also assumed that the MgO that will be emplaced in the repository will be present half as brucite and half as hydromagnesite; this assumption ensured that ample CO₂ was present without having to use a microbial reaction to titrate in CO₂.

In the second reaction (referred to as “run 2”), which consisted of just one step, we titrated NaOH into GWB and ERDA-6 with the compositions predicted at the invariant points at the end of run 1, step 2. The minerals present at the invariant points were also present at

the start of run 2. It is important to point out that run 2 does not in any way simulate reactions that are expected to occur in the repository. Rather, the objective of run 2 was to predict the compositions of brines with values of pCH higher than those expected so that LANL - CO personnel can synthesize brines for their experiments to determine the effects of the pCH on the speciation and solubilities of actinides. Because NaOH is often used to adjust the pCH in speciation and solubility experiments, we titrated it into GWB and ERDA-6 in run 2.

We used EQ6 in closed-system mode (model variable IOPT1 = 0) for run 1, step 2; and run 2. We suppressed (prevented from precipitating) the solids aragonite (CaCO_3), calcite (CaCO_3), dolomite ($\text{CaMg}(\text{CO}_3)_2$), hydromagnesite with the composition $\text{Mg}_4(\text{CO}_3)_3(\text{OH})_2 \cdot 3\text{H}_2\text{O}$, and nesquehonite ($\text{MgCO}_3 \cdot 3\text{H}_2\text{O}$) throughout run 1, steps 1 and 2; and run 2. We suppressed these phases to ensure that this analysis was consistent with the near-field chemical conceptual models (SCA, 2008; Brush and Xiong, 2011).

We used the EQ3/6 thermodynamic database (DB) DATA0.FM1 (Xiong, 2011) for this analysis. (DATA0.FM1 is in DATA0_FM1.ZIP, LIBEQ36, class DATABASES, in the CMS.) This DB differs from FMT_050405.CHEMDAT (Nowak, 2005; Xiong, 2005; LIBFMT, class CHEMDAT_2005), the DB used by Brush et al. (2009) to predict the solubilities of Th(IV), Np(V), and Am(III) for the CRA-2009 PABC, in that: (1) DATA0.FM1 contains an updated value of 0.392 for the Debye-Hückel slope of the osmotic coefficient A_ϕ (FMT still contains the old value of 0.39 because it is hard-wired into the code and cannot be changed without significant effort), and (2) DATA0.FM1 contains values of the dimensionless standard chemical potential (μ^0/RT) for both phase 3 ($\text{Mg}_2\text{Cl}(\text{OH})_3 \cdot 4\text{H}_2\text{O}$) and phase 5 ($\text{Mg}_3\text{Cl}(\text{OH})_5 \cdot 4\text{H}_2\text{O}$). (FMT_050405.CHEMDAT contains only phase 3.). Although Brush et al. (2009) used FMT_050405.CHEMDAT for the CRA-2009 PABC, laboratory studies of MgO at SNL in Carlsbad have shown that phase 5 precipitates from GWB instead of phase 3. Therefore, Xiong et al. (2009, 2010) determined μ^0/RT for phase 5, and Xiong (2009) added this value of μ^0/RT to FMT_050405.CHEMDAT and released FMT_090720.CHEMDAT (LIBFMT, class CHEMDAT_09072). Brush and Xiong (2011) provided a detailed history of the DBs used for WIPP compliance-related actinide-solubility calculations.

It was necessary to run EQ6 iteratively while adjusting the print interval to ensure that the code wrote output files (*.6o files) very close to each whole and half-unit of pCH (e.g., 7.0, 7.5, 8.0, etc). EQ6 uses a progress variable ξ , expressed in units of moles of titrants added to the brines, to track reactions. We determined that changing the ξ print interval (dlxprn), or the pH print interval (dlhprn), from their default value of 1.0×10^{38} to a value of 1.0×10^{-1} for dlxprn or 1.0×10^{-2} for dlhprn was sufficient to generate *.6o files close to the desired values of pCH.

We extracted the output from these EQ6 *.6o files by running the Excel macro "GetEQData.xls." This macro extracts all of the EQ6 output into an Excel spreadsheet; the 0.5 pCH print points were extracted using visual inspection.

All of the EQ3/6 input and output files used for this analysis, the Excel macro GetEQData.xls, and the Excel spreadsheets that contain the output extracted with GetEQData.xls are in the CMS in the zip file AP153Task1Data.zip in library LIBEQ36, class AP153.

The methods described above deviated in three ways from those described by Brush and Xiong (2011). First, Brush and Xiong (2011, Subsection 2.2.4) stated that:

We will use the FMT thermodynamic database FMT_090720.CHEMDAT, which contains both phase 3 and phase 5 ... and the equivalent EQ3/6 thermodynamic [DB] ... for the geochemical modeling to be performed for this AP.

However, we used DATA0.FM1 for this analysis instead of a DB equivalent to FMT_090720.CHEMDAT. DATA0.FM1 does indeed contain values of μ^0/RT for both phase 3 and phase 5. However, DATA0.FM1 contains an updated value of 0.392 for A_ϕ , but FMT still contains the old value of 0.39 (see above).

Second, we carried out titrations in run 1, step 2, and run 2 that were different from those anticipated by Brush and Xiong (2011, Subsection 4.1):

Task 1 will consist of using EQ6 for the following sequential reaction-path calculations: (1) reaction of the WIPP brines GWB and ERDA-6 ... with brucite from the hydration of all of the MgO emplaced in the repository, and with halite and anhydrite in the DRZ surrounding the repository (referred to as “step 1”); and (2) carbonation of brucite and phase 5 (GWB) or brucite (ERDA-6) to form hydromagnesite with the CO_2 produced by microbial consumption of all of the CPR [cellulosic, plastic, and rubber] materials in the repository by microbial denitrification and sulfate (SO_4^{2-}) reduction (“step 2”). The use of sequential EQ6 calculations (steps 1 and 2 above) is reasonable because the reactions in step 1 are fast with respect to the 10,000-year regulatory period, but those in step 2 are not. The use of sequential calculations is also consistent with the conceptual models for WIPP near-field chemistry and their implementation in PA

We added the organic ligands acetate, citrate, EDTA, and oxalate in run 1, step 1, which was inadvertently omitted from the description of step 1 in Brush and Xiong (2011, (Step 1 of Brush and Xiong (2009, Subsection 4.1) is essentially equivalent to run 1, steps 1 and 2, of this analysis.) Instead of titrating halite, anhydrite, and brucite into GWB and ERDA-6 in step 1 (Brush and Xiong, 2011, Subsection 4.1), we titrated halite, anhydrite, and brucite into these brines in run 1, step 2 and hydromagnesite was formed by carbonation of brucite. We did not titrate in CO_2 in either run 1 or 2, because we included 16 mM TIC in the initial brine compositions, which served as the CO_2 reservoir for these simulations. Because we did not titrate in CO_2 , we did not: (1) calculate “a molar quantity of CO_2 equal to that of the organic C in the CPR materials to be emplaced,” (2) “use spreadsheet calculations to scale the quantit[y] of ... CO_2 in the repository to 1 kg of H_2O for entry into the EQ3/6 input files,” or (3) “add a quantity of CO_2 equivalent to that produced by microbial consumption of all of the CPR materials in the repository without methanogenesis during step 2, instead of by simulating microbial SO_4^{2-} reduction directly” (Brush and Xiong, 2011, Subsection 4.1).

Third, although we did include $\text{ThO}_2(\text{am})$, KNpO_2CO_3 , and $\text{Am}(\text{OH})_3(\text{s})$ to simulate the presence of actinide-bearing solids, we did not “compare their final, equilibrium solubilities to those predicted by FMT.” This is because the DB used for this analysis, DATA0.FM1, is not equivalent to FMT_050405.CHEMDAT the FMT DB used to predict the solubilities of Th(IV), Np(V), and Am(III) for the CRA-2009 PABC, or FMT_090720.CHEMDAT (see above).

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3 RESULTS

Table 2 provides the following information for GWB: (1) its initial (prior to run 1, step 1) composition (this composition was established by Krumhansl et al., 1991; and Snider, 2003; not by our EQ3/6 modeling); (2) its predicted composition and other parameters, such as f_{CO_2} , pcH, and TIC, during run 1, step 2 (pcH = 7.00, 7.50, ..., 9.00); (3) its predicted composition after run 1, step 2 (pcH = 9.4268); (4) its predicted composition during run 2 (pcH = 9.50, 10.0, ..., 13.0); and (5) its predicted composition after run 2 (pcH = 13.2098). Table 3 provides comparable information for ERDA-6. (Popielak et al., 1983, established the initial composition of ERDA-6). Tables 2 and 3 predict the compositions for GWB and ERDA-6 from pcH = 7.00 to 13.2, a range of 6.2 units.

It is worth noting that, despite our efforts to set the EQ6 print interval such that the code wrote *.60 files very close to each whole or half-unit of pcH, the code wrote output files for predicted pcH values that deviated slightly from the desired values of whole- or half-units after rounding to three significant figures (e.g., the code wrote *.60 files for values that sometimes deviated by 0.01 unit).

It is also worth noting that the compositions and other parameters predicted for these brines are generally, but not always, different after runs 1 and 2, despite the fact that the same titrants were used for both brines. This is to be expected, given that the initial compositions of GWB and ERDA-6 are quite different.

Again, we maintain that the compositions and values of other parameters predicted for GWB and ERDA-6 after run 1, step 2, should not be compared to the values predicted for the same invariant points with FMT by Brush et al. (2009) for the Th(IV), Np(V), and Am(III) solubility calculations for the CRA-2009 PABC. This is because the thermodynamic DBs used for these calculations (DATA0.FM1 and FMT_050405.CHEMDAT, respectively) are not equivalent (see Section 2 above).

Finally, these results show that there is at least one prediction that agrees with experimentally observed results. The total dissolved Mg concentration of GWB increases from its initial value of 1.02 M (Krumhansl et al., 1991; Snider, 2003) to 1.20 M at pcH = 9.00; decreases to 0.44 M after run 1, step 2, and 0.359 M at pcH = 9.50; and then drops rapidly beginning at pcH = 10.0 (see Table 2). Similarly, the Mg(II)(aq) concentration of ERDA-6 increases from its initial value of 0.019 M (Popielak et al., 1983) to 0.135 M at pcH = 9.50 and 9.69 (after run 1, step 1), and then drops sharply beginning at pcH = 10.0 (Table 3). These rapid decreases in the Mg concentration predicted by EQ3/6 are consistent with the formation of large quantities of solids in these brines in lab experiments that increase the pcH to the “cloud point” at pcH values slightly above those expected in the WIPP.

Table 2. Composition of GWB (M Unless Otherwise Noted) and Other Parameters (Units as Noted) during Reactions with Solids and NaOH.

| Element or Property | Initial Composition of GWB ^A | pcH = 7.00 ^B | pcH = 7.50 | pcH = 8.00 |
|-----------------------------------|---|-------------------------|-----------------------|-----------------------|
| B(III)(aq) | 0.158 | 0.158 | 0.158 | 0.158 |
| Na(I)(aq) | 3.53 | 3.29 | 3.26 | 3.26 |
| Mg(II)(aq) | 1.02 | 1.12 | 1.15 | 1.17 |
| K(I)(aq) | 0.467 | 0.474 | 0.468 | 0.467 |
| Ca(II)(aq) | 0.014 | 0.00830 | 0.00829 | 0.00854 |
| S(VI)(aq) | 0.177 | 0.184 | 0.186 | 0.186 |
| Cl(-I)(aq) | 5.86 | 5.62 | 5.60 | 5.59 |
| Br(-I)(aq) | 0.0266 | 0.0266 | 0.0266 | 0.0266 |
| f _{CO₂} (atm) | ND ^C | 6.61×10^{-6} | 6.61×10^{-6} | 6.61×10^{-6} |
| I (m) | ND ^C | 8.40 | 8.40 | 8.41 |
| pH ^D | ND ^C | 5.78 | 6.28 | 6.78 |
| pcH ^E | ND ^C | 7.0003 ^D | 7.4963 ^D | 7.9965 ^D |
| RH (%) ^F | ND ^C | 71.5 | 71.5 | 71.5 |
| TIC | ND ^C | 8.23×10^{-7} | 1.63×10^{-6} | 5.98×10^{-6} |

Table 2 continued on next page. Footnotes provided on last two pages of Table 2

Table 2. Composition of GWB (M Unless Otherwise Noted) and Other Parameters (Units as Noted) during Reactions with Solids and NaOH (cont.).

| Element or Property | pcH = 8.50 ^B | pcH = 9.00 ^B | Composition of GWB after run 1, step 2 ^G | pcH = 9.50 ^H |
|-----------------------------------|-------------------------|-------------------------|---|-------------------------|
| B(III)(aq) | 0.158 | 0.158 | 0.184 | 0.175 |
| Na(I)(aq) | 3.25 | 3.25 | 4.11 | 4.56 |
| Mg(II)(aq) | 1.18 | 1.20 | 0.440 | 0.359 |
| K(I)(aq) | 0.467 | 0.467 | 0.544 | 0.516 |
| Ca(II)(aq) | 0.00893 | 0.00939 | 0.0134 | 0.0121 |
| S(VI)(aq) | 0.186 | 0.187 | 0.223 | 0.211 |
| Cl(-I)(aq) | 5.59 | 5.58 | 4.91 | 5.20 |
| Br(-I)(aq) | 0.0266 | 0.0266 | 0.0310 | 0.0294 |
| f _{CO₂} (atm) | 6.62 × 10 ⁻⁶ | 6.62 × 10 ⁻⁶ | 3.14 × 10 ⁻⁶ | 3.14 × 10 ⁻⁶ |
| I (m) | 8.41 | 8.40 | 6.93 | 7.19 |
| pH ^D | 7.28 | 7.78 | 8.49 | 8.49 |
| pcH ^E | 8.4974 | 8.9989 | 9.4268 | 9.4973 |
| RH (%) ^F | 71.6 | 71.6 | 76.3 | 74.6 |
| TIC | 3.37 × 10 ⁻⁵ | 2.58 × 10 ⁻⁴ | 3.72 × 10 ⁻⁴ | 3.77 × 10 ⁻⁴ |

Table 2 continued on next page. Footnotes provided on last two pages of Table 2

Table 2. Composition of GWB (M Unless Otherwise Noted) and Other Parameters (Units as Noted) during Reactions with Solids and NaOH (cont.).

| Element or Property | pcH = 10.00 ^H | pcH = 10.50 ^H | pcH = 11.00 ^H | pcH = 11.50 ^H |
|-----------------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| B(III)(aq) | 0.157 | 0.157 | 0.157 | 0.157 |
| Na(I)(aq) | 5.31 | 5.39 | 5.40 | 5.40 |
| Mg(II)(aq) | 0.0446 | 0.00559 | 6.22×10^{-4} | 7.09×10^{-5} |
| K(I)(aq) | 0.465 | 0.465 | 0.465 | 0.465 |
| Ca(II)(aq) | 0.0148 | 0.0186 | 0.0198 | 0.0200 |
| S(VI)(aq) | 0.188 | 0.184 | 0.183 | 0.183 |
| Cl(-I)(aq) | 5.33 | 5.33 | 5.33 | 5.33 |
| Br(-I)(aq) | 0.0265 | 0.0265 | 0.0265 | 0.0265 |
| f _{CO₂} (atm) | 3.14×10^{-6} | 2.69×10^{-6} | 2.67×10^{-7} | 2.66×10^{-8} |
| I (m) | 7.02 | 7.00 | 7.01 | 7.01 |
| pH ^D | 8.99 | 9.50 | 10.0 | 10.5 |
| pcH ^E | 9.9964 | 10.4985 | 10.9989 | 11.499 |
| RH (%) ^F | 74.1 | 74.1 | 74.1 | 74.1 |
| TIC | 7.23×10^{-4} | 3.01×10^{-3} | 2.46×10^{-3} | 2.34×10^{-3} |

Table 2 continued on next page. Footnotes provided on last two pages of Table 2

Table 2. Composition of GWB (M Unless Otherwise Noted) and Other Parameters (Units as Noted) during Reactions with Solids and NaOH (cont.).

| Element or Property | | | | Composition of |
|-----------------------------------|--------------------------|--------------------------|--------------------------|------------------------------|
| | pcH = 12.00 ^H | pcH = 12.50 ^H | pcH = 13.00 ^H | GWB after run 2 ^I |
| B(III)(aq) | 0.157 | 0.157 | 0.157 | 0.157 |
| Na(I)(aq) | 5.40 | 5.40 | 5.41 | 5.41 |
| Mg(II)(aq) | 9.64×10^{-6} | 1.77×10^{-6} | 4.33×10^{-7} | 2.51×10^{-7} |
| K(I)(aq) | 0.465 | 0.465 | 0.465 | 0.465 |
| Ca(II)(aq) | 0.0201 | 0.0202 | 0.0205 | 0.0208 |
| S(VI)(aq) | 0.183 | 0.183 | 0.182 | 0.182 |
| Cl(-I)(aq) | 5.33 | 5.32 | 5.32 | 5.31 |
| Br(-I)(aq) | 0.0265 | 0.0265 | 0.0265 | 0.0265 |
| f _{CO₂} (atm) | 2.66×10^{-9} | 2.54×10^{-10} | 2.65×10^{-11} | 9.85×10^{-12} |
| I (m) | 7.01 | 7.01 | 7.02 | 7.02 |
| pH ^D | 11.0 | 11.5 | 12.0 | 12.2 |
| pcH ^E | 11.9989 | 12.4985 | 12.9971 | 13.2098 |
| RH (%) ^F | 74.1 | 74.1 | 74.1 | 74.1 |
| TIC | 0.00230 | 0.00229 | 0.00228 | 0.00227 |

- A. Composition of GWB prior to reactions with solids (Krumhansl et al., 1991; Snider, 2003).
 B. Added acetate, citrate, EDTA, and oxalate to GWB in run 1, step 1. Titrated in halite, anhydrite, brucite, hydromagnesite, ThO₂(am), KNpO₂CO₃(s), and Am(OH)₃(s) in run 1, step 2. These results are from run 1, step 2.
 C. Not determined by Krumhansl et al. (1991) or Snider (2003).

Footnotes for Table 2 continued on next page

Footnotes for Table 2 (continued)

- D. National Bureau of Standards (NBS) pH scale.
 - E. The values of the pcH predicted by EQ3/6 were not rounded to three significant figures to show how close our setting of the pcH print interval came to generating output at each whole and half-unit of pcH (e.g., 7.00, 7.50, etc).
 - F. The value of the RH predicted by EQ3/6 divided by 100 yields the value of the activity of H₂O in GWB.
 - G. Composition of GWB after complete reaction with halite, anhydrite, brucite, hydromagnesite, ThO₂(am), KNpO₂CO₃(s), and Am(OH)₃(s).
 - H. Titrated in NaOH in run 2. Did not titrate in the solids added in run 1, step 2 (halite, anhydrite, brucite, hydromagnesite, and the actinide-bearing solids), because sufficient quantities of these phases left over from run 1, step 2, to maintain equilibrium between the brines and these solids.
 - I. Composition of GWB after complete reaction with NaOH.
-

Table 3. Composition of ERDA-6 (M Unless Otherwise Noted) and Other Parameters (Units as Noted) during Reactions with Solids and NaOH.

| Element or Property | Initial Composition of ERDA-6 ^A | pcH = 7.00 ^B | pcH = 7.50 ^B | pcH = 8.00 ^B |
|-----------------------------------|--|-------------------------|-------------------------|-------------------------|
| B(III)(aq) | 0.063 | 0.0627 | 0.0626 | 0.0627 |
| Na(I)(aq) | 4.871 | 4.89 | 4.93 | 4.94 |
| Mg(II)(aq) | 0.019 | 0.0774 | 0.106 | 0.113 |
| K(I)(aq) | 0.097 | 0.117 | 0.0994 | 0.0968 |
| Ca(II)(aq) | 0.012 | 0.0119 | 0.0117 | 0.0119 |
| S(VI)(aq) | 0.17 | 0.183 | 0.185 | 0.186 |
| Cl(-I)(aq) | 4.8 | 4.82 | 4.86 | 4.87 |
| Br(-I)(aq) | 0.011 | 0.0109 | 0.0109 | 0.0109 |
| f _{CO₂} (atm) | ND ^C | 7.16 × 10 ⁻⁶ | 7.13 × 10 ⁻⁶ | 7.12 × 10 ⁻⁶ |
| I (m) | ND ^C | 6.19 | 6.27 | 6.29 |
| pH ^D | 6.17 | 6.13 | 6.61 | 7.11 |
| pcH ^E | ND ^C | 7.0049 | 7.4997 | 8.0008 |
| RH (%) ^F | ND ^C | 77.4 | 77.1 | 77.1 |
| TIC | 0.016 | 1.06 × 10 ⁻⁶ | 2.07 × 10 ⁻⁶ | 5.74 × 10 ⁻⁶ |

Table 3 continued on next page. Footnotes provided on last two pages of Table 3

Table 3. Composition of ERDA-6 (M Unless Otherwise Noted) and Other Parameters (Units as Noted) during Reactions with Solids and NaOH (continued).

| Element or Property | pcH = 8.50 ^B | pcH = 9.00 ^B | pcH = 9.50 ^B | Composition of ERDA-6 after run 1, step 2 ^G |
|-----------------------------------|-------------------------|-------------------------|-------------------------|--|
| B(III)(aq) | 0.0626 | 0.0626 | 0.0626 | 0.0621 |
| Na(I)(aq) | 4.94 | 4.95 | 4.96 | 5.30 |
| Mg(II)(aq) | 0.119 | 0.126 | 0.135 | 0.135 |
| K(I)(aq) | 0.0965 | 0.0964 | 0.0964 | 0.0956 |
| Ca(II)(aq) | 0.0123 | 0.0128 | 0.0135 | 0.0116 |
| S(VI)(aq) | 0.186 | 0.187 | 0.187 | 0.182 |
| Cl(-I)(aq) | 4.87 | 4.88 | 4.88 | 5.24 |
| Br(-I)(aq) | 0.0109 | 0.0109 | 0.0109 | 0.0108 |
| f _{CO₂} (atm) | 7.12 × 10 ⁻⁶ | 7.11 × 10 ⁻⁶ | 7.11 × 10 ⁻⁶ | 3.14 × 10 ⁻⁶ |
| I (m) | 6.31 | 6.34 | 6.36 | 6.80 |
| pH ^D | 7.61 | 8.11 | 8.61 | 8.69 |
| pcH ^E | 8.502 | 9.0037 | 9.5056 | 9.6911 |
| RH (%) ^F | 77.0 | 77.0 | 76.9 | 74.7 |
| TIC | 2.00 × 10 ⁻⁵ | 9.10 × 10 ⁻⁵ | 5.81 × 10 ⁻⁴ | 4.55 × 10 ⁻⁴ |

Table 3 continued on next page. Footnotes provided on last two pages of Table 3

Table 3. Composition of ERDA-6 (M Unless Otherwise Noted) and Other Parameters (Units as Noted) during Reactions with Solids and NaOH (continued).

| Element or Property | pcH = 10.00 ^H | pcH = 10.50 ^H | pcH = 11.00 ^H | pcH = 11.50 ^H |
|-----------------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| B(III)(aq) | 0.0621 | 0.0621 | 0.0621 | 0.0621 |
| Na(I)(aq) | 5.48 | 5.54 | 5.55 | 5.55 |
| Mg(II)(aq) | 3.64×10^{-2} | 4.39×10^{-3} | 4.82×10^{-4} | 5.56×10^{-5} |
| K(I)(aq) | 0.0956 | 0.0956 | 0.0956 | 0.0956 |
| Ca(II)(aq) | 0.0132 | 0.0155 | 0.0161 | 0.0162 |
| S(VI)(aq) | 0.173 | 0.169 | 0.169 | 0.169 |
| Cl(-I)(aq) | 5.24 | 5.23 | 5.23 | 5.23 |
| Br(-I)(aq) | 0.0108 | 0.0108 | 0.0108 | 0.0108 |
| f _{CO₂} (atm) | 3.14×10^{-6} | 2.31×10^{-6} | 2.3E-07 | 2.30×10^{-8} |
| I (m) | 6.69 | 6.66 | 6.66 | 6.66 |
| pH ^D | 9.01 | 9.52 | 10.0 | 10.52 |
| pcH ^E | 9.996 | 10.4975 | 10.9977 | 11.4977 |
| RH (%) ^F | 74.8 | 74.9 | 74.9 | 74.9 |
| TIC | 7.85×10^{-4} | 3.00×10^{-3} | 2.52×10^{-3} | 2.41×10^{-3} |

Table 3 continued on next page. Footnotes provided on last two pages of Table 3

Table 3. Composition of ERDA-6 (M Unless Otherwise Noted) and Other Parameters (Units as Noted) during Reactions with Solids and NaOH (continued).

| Element or Property | pcH = 12.00 ^H | pcH = 12.50 ^H | pcH = 13.00 ^H | Composition of ERDA-6 after run 2 ^I |
|-----------------------------------|--------------------------|--------------------------|--------------------------|--|
| B(III)(aq) | 0.0621 | 0.0621 | 0.0621 | 0.0621 |
| Na(I)(aq) | 5.55 | 5.55 | 5.56 | 5.56 |
| Mg(II)(aq) | 7.84×10^{-6} | 1.50×10^{-6} | 3.78×10^{-7} | 2.39×10^{-7} |
| K(I)(aq) | 0.0956 | 0.0956 | 0.0956 | 0.0956 |
| Ca(II)(aq) | 0.0162 | 0.0163 | 0.0166 | 0.0169 |
| S(VI)(aq) | 0.169 | 0.169 | 0.168 | 0.168 |
| Cl(-I)(aq) | 5.23 | 5.23 | 5.22 | 5.22 |
| Br(-I)(aq) | 0.0108 | 0.0108 | 0.0108 | 0.0108 |
| f _{CO₂} (atm) | 2.30×10^{-9} | 2.29×10^{-10} | 2.28×10^{-11} | 9.85×10^{-12} |
| I (m) | 6.66 | 6.67 | 6.67 | 6.68 |
| pH ^D | 11.0 | 11.5 | 12.0 | 12.2 |
| pcH ^E | 11.9975 | 12.497 | 12.9956 | 13.1762 |
| RH (%) ^F | 74.9 | 74.9 | 74.8 | 74.8 |
| TIC | 2.37×10^{-3} | 2.36×10^{-3} | 2.35×10^{-3} | 2.34×10^{-3} |

A. Composition of ERDA-6 prior to reaction 1, step 1 (Popielak et al., 1983).

B. Added acetate, citrate, EDTA, and oxalate to ERDA-6 in run 1, step 1. Titrated in halite, anhydrite, brucite, hydromagnesite, ThO₂(am), KNpO₂CO₃(s), and Am(OH)₃(s) in run 1, step 2. These results are from run 1, step 2.

C. Not determined by Popielak et al. (1983).

Footnotes for Table 3 continued on next page

Footnotes for Table 3 (continued)

- D. National Bureau of Standards (NBS) pH scale.
 - E. The values of the pcH predicted by EQ3/6 were not rounded to three significant figures to show how close our setting of the pcH print interval came to generating output at each whole and half-unit of pcH (e.g., 7.00, 7.50, etc).
 - F. The value of the RH predicted by EQ3/6 divided by 100 yields the value of the activity of H₂O in ERDA-6.
 - G. Composition of ERDA-6 after complete reaction with halite, anhydrite, brucite, hydromagnesite, ThO₂(am), KNpO₂CO₃(s), and Am(OH)₃(s).
 - H. Titrated in NaOH in run 2. Did not titrate in the solids added in run 1, step 2 (halite, anhydrite, brucite, hydromagnesite, and the actinide-bearing solids), because sufficient quantities of these phases were left over from run 1, step 2, to maintain equilibrium between the brines and these solids.
 - I. Composition of ERDA-6 after complete reaction with NaOH.
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4 CONCLUSIONS

This analysis report provides the results of our predictions of the compositions of the standard WIPP brines GWB and ERDA-6 during and after reactions with the solids in WIPP disposal rooms, and during and after reactions with NaOH and solids in the repository. We will provide these compositions to LANL — CO personnel so that they can use these them to synthesize brines for experiments to determine the effects of the pcH on the speciation and solubilities of actinide elements in the repository (Lucchini et al., 2007; Borkowski et al., 2009; Borkowski, 2010). We used EQ3/6, Version 8.0a (Wolery and Jarek, 2003; Wolery, 2008; Wolery et al., 2010) for this analysis, which we carried out under Task 1 of AP-153 (Brush and Xiong, 2011).

Tables 2 and 3 (see Section 3 above) provide the following information for GWB and ERDA-6: (1) their initial compositions (Krumhansl et al., 1991; Snider, 2003; Popielak et al. 1983); (2) their predicted compositions and other parameters, such as f_{CO_2} , pcH, and TIC, during reactions with the solids specified in the conceptual models for WIPP near-field chemistry; (3) their predicted compositions after equilibration with these solids; (4) their predicted compositions during reactions with NaOH and solids; and (5) their predicted compositions after equilibration with NaOH and solids.

After equilibration with the solids specified in the conceptual models for near-field chemistry, the predicted brine compositions define so-called invariant points (one each for GWB and ERDA-6), because the solids — especially brucite and hydromagnesite — control the new compositions of the brines and parameters such as f_{CO_2} , pH, and TIC. However, the reactions among NaOH, brines, and solids do not in any way simulate reactions that are expected to occur in the repository. Rather, the objective of adding NaOH to the brines was to predict their compositions at values of pcH higher than those expected so that LANL – CO personnel can synthesize them for experiments to determine the effects of the pcH on the speciation and solubilities of actinides.

Tables 2 and 3 (Section 3) predict the compositions for GWB and ERDA-6 from pcH = 7.00 to 13.2, a range of 6.2 units.

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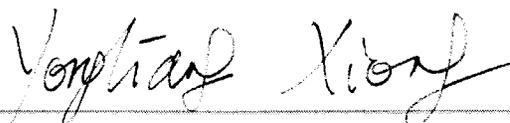
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