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*Title:* PHREEQC Calculations of Geochemical Speciation in Groundwater, in Support of the "Well Screen Analysis Report Revision 2"

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# PHREEQC CALCULATIONS OF GEOCHEMICAL SPECIATION IN GROUNDWATER, IN SUPPORT OF THE "*WELL SCREEN ANALYSIS REPORT REVISION 2*"

## 1. PURPOSE

The purpose of these modeling calculations is to determine the dominant geochemical speciation of selected solutes (dissolved species) in native groundwater. Geochemical speciation determines fate and transport characteristics of these analytes, such as adsorption onto charged mineral surfaces and mineral solubility limits. These calculations help to establish the technical basis for identifying which analytes may be affected by residual drilling impacts and for selecting suitable geochemical indicators for those impacts. Results of these speciation calculations are used in the *Well Screen Analysis Report Revision 02* (LANL 2007, ER-ID to be determined).

## 2. SCOPE

The scope of these calculations covers general chemical analytes that are commonly used to characterize groundwater quality, as well as trace elements (e.g., phosphate, bromide, and arsenic) and trace metals (e.g., uranium, iron, and manganese) in groundwater considered representative of background conditions in perched intermediate zones and the regional aquifer beneath the Pajarito Plateau. Although they are not detected in background groundwaters, several additional trace metals and radionuclides are included in the model input simply to determine their dominant speciation.

These calculations are not intended to replace detailed geochemical evaluations such as those presented in characterization well geochemistry reports. Rather, they provide transparent and consistent modeling calculations of the speciation of solutes that are (or could be) present in representative groundwater under predrilling conditions.

## 3. SOFTWARE

Geochemical speciation is calculated using the computer code PHREEQC (Parkhurst and Appelo 1999, 095402) for the inorganic analytes selected as relevant to this report. The speciation model calculations are run using the following thermodynamic databases:

- *MINTEQ.DAT*, derived from the database files of MINTEQA2 (Allison et al 1991, 049930),
- *WATEQ.V4.dat*, which is essentially the same as WATEQ4F (Ball and Nordstrom 1991), and
- Yucca Mountain Project (YMP) database, *phreeqcDATA025.dat*, used for radionuclide and trace-metal species that were not in the WATEQ.V4 database. The YMP PHREEQC database is a translation of the YMP EQ3/6 thermodynamic database into a format that can be used by PHREEQC. The thermodynamic data in the YMP EQ3/6 database was evaluated and qualified by BSC (2004).

The databases *MINTEQ.DAT* and *WATEQ.V4.dat* are accessible for downloading along with the PHREEQC program from the U.S. Geological Survey's website, (http://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqc/index.html).

## 4. INPUT DATA

For naturally-occurring chemical species, including trace metals, input concentrations for the model are taken from the "Groundwater Background Investigation Report Revision 02" (LANL 2007, 094856, Tables 4.2-2 and 4.2-3). In Appendix A, Tables A-1 and A-2 list median and upper limits for background concentrations for the constituents included in the model input.

For most of the radioactive elements, input concentrations for the model are arbitrarily set at 0.001 mg/L. This was the case for americium, cerium, cesium, neptunium, plutonium, and technetium. Although these concentrations are much higher than could be reasonably expected, this input is only used for the purposes of speciation and not for mineral saturation. Radioactive isotopes of cobalt, strontium, and

uranium are assumed to exhibit the same geochemical speciation as that of the total element included in the input file. Geochemical speciation of radiogenic and stable isotopes of a given element are assumed to be the same regardless of the half-life or mode of decay. For example, under alkaline pH and oxidizing conditions, the speciation of uranium-238, uranium-235, and uranium-234 is identical to that of total or natural uranium.

## 5. APPROACH

The base case for geochemical speciation in groundwater uses median concentrations for the regional aquifer, together with 0.001 mg/L specified for radionuclides not occurring naturally in the groundwater (Tables A-1 and A-2). The temperature for the model is specified as 25°C. The prevailing electrochemical potential for the base case is specified as $E_H$ = 533 mV, corresponding to pe = 9.0. This redox potential is approximately that which would be expected for groundwater in equilibrium with manganese dioxide and was selected as the redox state most consistent with the following geochemical observations:

- ubiquitous presence of oxidized forms of dissolved iron (ferric), nitrogen (nitrate), sulfur (sulfate), uranium (uranyl), and dissolved oxygen,
- presence of manganese dioxide and ferric (oxy)hydroxide in borehole geologic samples,
- absence of dissolved native sulfide and sulfide minerals,
- low dissolved concentrations of iron and manganese (less than 0.01 mg/L), and
- detection of species that are stable in oxidized forms, including perchlorate, chromate, molybdate, and uranium(VI), in groundwater at the Laboratory

The extent to which speciation calculations for the base case are also applicable to other geochemical conditions within the range of background concentrations is tested by running a series of bounding cases, as follows:

- upper tolerance limits (UTL) or maximum concentration for a given analyte within the regional aquifer
- median concentrations for the intermediate perched zones
- UTL or maximum concentration for a given analyte within intermediate perched zones

Finally, to identify those species whose dominant oxidation state and speciation could change significantly under reducing conditions, cases using the median concentrations of the regional aquifer and the intermediate perched zone are rerun specifying Eh = -260 mV (pe = -4.4) at 25°C. This redox potential corresponds to the $HCO_3^-/CH_4(g)$ redox couple at pH 7 and 25°C, and simulates methanogenic conditions in groundwater.

Key input parameters for each of these six modeling cases are summarized in Table 5-1:

**Table 5-1. Key Input Parameters for PHREEQC modeling cases**

| Modeling Case | pH | Alkalinity (mg/L as $CO_3$) | Eh (mV) | pe | Concentrations of Dissolved Species |
|---|---|---|---|---|---|
| Base Case | 7.82 | 67.67 | 533 | 9.0 | Median concentrations, regional aquifer (Table A-1) |
| Bounding case 1 | 8.65 | 129.8 | 533 | 9.0 | Upper limits, regional aquifer (Table A-1) |
| Bounding case 2 | 7.39 | 46.14 | 533 | 9.0 | Median concentrations, intermediate perched zone (Table A-2) |
| Bounding case 3 | 8.80 | 62.4 | 533 | 9.0 | Upper limits, intermediate perched zone (Table A-2) |
| Bounding case 4 | 7.82 | 67.67 | -260 | -4.4 | Median concentrations, regional aquifer (Table A-1) |
| Bounding case 5 | 7.39 | 46.14 | -260 | -4.4 | Median concentrations, intermediate perched zone (Table A-2) |

## 6. RESULTS

Dominant oxidation states and speciation results for dissolved species are presented in Appendix B for the six cases listed above, with summary tables presented in this section.

Base case. Table 6-1 summarizes the detailed speciation results for the base case according to the nature of the dominant dissolved species for each element: its charge state and complexing species:

- For 39 of the 44 elements (89%) included in the base case, a single species accounts for 75% or more of the total dissolved concentration for that element.
- Secondary species that comprise more than 25% of the total element concentration are predicted to be present only for five elements: Be, Fe, Ce, Np, and Pu.
- Twenty-two (50%) of the 44 elements are present predominately as cations.

**Table 6-1. Dominant geochemical speciation for base case**

| Dissolved species | Neutral (uncharged) | Cation | Anion | Category[a] total |
|---|---|---|---|---|
| Free ion | — | Ba, Cd, Ca, Cs, Co, Li, Mg, Mn, Ni, K, Ag, Na, Ra, Sr, Tl, Zn | Br, Cl, F | *Primary: 19*<br>*Secondary: —* |
| Oxide species | — | Np, Pu | Sb, As, Cr, Mo, N, P, Se, S, V, Tc | *Primary: 12*<br>*Secondary —* |
| Hydroxide species | B, (Be), (Fe), Hg, Si | Be, Fe | Al, Sn | *Primary: 7*<br>*Secondary: 2* |
| Carbonate species | Cu, Pb | Am, Ce | C, (Ce), (Np), (Pu), U | *Primary: 6*<br>*Secondary: 3* |
| *Category[a] total* | *Primary: 5*<br>*Secondary: 2* | *Primary: 22*<br>*Secondary: —* | *Primary: 17*<br>*Secondary: 3* | *Primary: 44*<br>*Secondary: 5* |

Source: Table B-1

[a] Primary species are those accounting for the largest proportion of the total elemental concentration. Elements shown in parentheses indicate species that are secondary in dominance but that contribute more than 25% to the total elemental concentration.

Of particular interest is the distribution of species for the 25 dissolved trace metals (present only at submilligram concentrations) and 7 radioactive elements:

- Slightly more than one-third of the trace metals and radionuclide elements are present as free (uncomplexed) cations (12 out of 32, or 38%).
- A slightly smaller proportion are present as negatively-charged anions (10 out of 32, or 31%), predominantly as oxyanions, as well as a very few hydroxide and carbonate complexes.
- Six of the metal and radionuclide elements (19% of 32) are dominated by cationic complexes.
- The remaining four trace elements (B, Hg, Cu, Pb) are dominated by neutral species (12% of 32).

Tables 6-2 though 6-6 summarize dominant speciation for each of the five bounding cases. General observations are made by contrasting the results for each bounding case against those for the base case.

Bounding case 1. Upper limits for background levels in the regional aquifer. Two major shifts are evident when concentrations are increased to their upper background levels (Table 6-2).

First, the proportion of elements for which a single species accounts for 75% or more of the total dissolved concentration decreases to 33 out of 44 (75%, compared to 89% for the base case), as complexed species increase in relative importance for metals and alkaline earths. The number of elements for which secondary species comprise more than 25% of the total element concentration more than doubles in this bounding case, with secondary species listed for 11 elements (25% of 44): Be, Cd, Co, Fe, Ni, Zn, Am, Ce, Cs, Np, and Pu.

Secondly, a much smaller proportion of the elements (14 out of 44, or 32%) are dominated by cationic species, compared to 50% for the base case. All of the elements in this category are dominated by their free (uncomplexed) form; cationic complexes are not the dominant species for any of the elements considered.

Among the 32 trace metals and radionuclides:

- Ten (31% of 32) are dominated by free cations, compared to 12 (38%) in the base case.
- Eight elements that were dominated by cationic species for the base case shift to being dominated by neutral hydroxide complexes (Be, Fe), neutral carbonate complexes (Ni, Zn), or anionic carbonate complexes (Am, Ce, Np, Pu).
- Altogether, 14 are predominantly anions (44% of 32), of which 7 are oxyanions, 5 are carbonate complexes, and 2 are hydroxide complexes.

**Table 6-2. Dominant geochemical speciation for bounding case 1**

| Dissolved species | Neutral (uncharged) | Cation | Anion | Category[a] total |
|---|---|---|---|---|
| Free ion | — | Ba, Cd, Ca, Cs, Co, Li, Mg, Mn, (Ni), K, Ag, Na, Ra, Sr, Tl, (Zn) | Br, Cl, F | *Primary:* 17<br>*Secondary:* 2 |
| Oxide species | — | (Np), (Pu) | Sb, As, Cr, Mo, N, P, Se, S, V, Tc | *Primary:* 10<br>*Secondary:* 2 |
| Hydroxide species | B, Be, Fe, Hg, Si | (Am), (Be) | Al, (Fe), Sn | *Primary:* 7<br>*Secondary:* 3 |
| Carbonate species | (Cd), (Co), Cu, Ni, Pb, (Pu), Zn | (Am) | Am, C, Ce, Np, Pu, U | *Primary:* 10<br>*Secondary:* 4 |
| *Category[a] total* | *Primary:* 9<br>*Secondary:* 3 | *Primary:* 14<br>*Secondary:* 7 | *Primary:* 21<br>*Secondary:* 1 | *Primary:* 44<br>*Secondary:* 11 |

Source: Table B-2

[a] Primary species are those accounting for the largest proportion of the total elemental concentration. Elements shown in parentheses indicate species that are secondary in dominance but that account for more than 25% of the total elemental concentration.

Underlined species indicate differences relative to base case speciation.

Bounding case 2. Median concentrations for the intermediate perched zone. With the exception of U, the dominant speciation in groundwater from the intermediate perched zone (Table 6-3) is identical to that for the base case. The major noticeable difference is that no secondary species are listed for this bounding case; in contrast, for the base case, five elements had secondary species. This shift is due to the fact that the median alkalinity in the intermediate perched zone (38.45 mg/L as $CaCO_3$) is only 58% of that in the regional aquifer (66 mg/L as $CaCO_3$), such that the significance of carbonate species is somewhat diminished and that of other species becomes more prominent. Also as a result of lower alkalinity for this bounding case, the anionic uranyl phosphate complex becomes the dominant species predicted for U in this groundwater.

**Table 6-3. Dominant geochemical speciation for bounding case 2**

| Dissolved species | Neutral (uncharged) | Cation | Anion | Category[a] total |
|---|---|---|---|---|
| Free ion | — | Ba, Cd, Ca, Cs, Co, Li, Mg, Mn, Ni, K, Ag, Na, Ra, Sr, Tl, Zn | Br, Cl, F | *Primary:* 19<br>*Secondary:* — |
| Oxide species | — | Np, Pu | Sb, As, Cr, Mo, N, P, Se, S, V, Tc | *Primary:* 12<br>*Secondary:* — |
| Hydroxide species | B, Hg, Si | Be, Fe | Al, Sn | *Primary:* 7<br>*Secondary:* — |
| Carbonate species | Cu, Pb | Am, Ce | C | *Primary:* 5<br>*Secondary:* — |
| Phosphate species | — | — | U | *Primary:* 1<br>*Secondary:* — |
| *Category[a] total* | *Primary:* 5<br>*Secondary:* — | *Primary:* 22<br>*Secondary:* — | *Primary:* 17<br>*Secondary:* — | *Primary:* 44<br>*Secondary:* — |

Source: Table B-3

[a] Primary species are those accounting for the largest proportion of the total elemental concentration. Elements shown in parentheses indicate species that are secondary in dominance but that account for more than 25% of the total elemental concentration.

Underlined species indicate differences relative to base case speciation. Although the dominant species for Be, Fe, Ce and Pu are the same in this bounding as for the base case, these species are underlined to indicate the diminished contribution of the secondary species that are marked as such in the base case (Table 6-1).

Bounding case 3. Upper concentration limits for the intermediate perched zone. The UTL for alkalinity in the intermediate perched zone (52 mg/L as $CaCO_3$) is 79% of the median alkalinity in the regional aquifer (66 mg/L as $CaCO_3$), as compared to 58% for median alkalinity in the perched zone for the previous bounding case. Nonetheless, speciation calculations for this bounding case (Table 6-4) are less similar to that for the base case than was obtained using median concentrations values (Table 6-3). The increased contrast is due to the fact that the UTL for pH is one pH unit higher in the perched zone (8.80) than in the base case (7.82). As a result of the higher pH and alkalinity, hydroxide and carbonate complexes become more prominent than in the previous bounding case, in primary as well as secondary categories of importance.

- For 35 of the 44 elements (80%), a single species accounts for 75% or more of the total dissolved concentration for that element.
- Secondary species that comprise more than 25% of the total element concentration are predicted to be present for nine elements: Am, B, Cd, Co, Fe, Ni, Pb, Pu, and Zn. Although secondary species are listed for five elements in the base case, Fe and Pu are the only elements in common between the two lists.
- Fifteen (34%) of the 44 elements are present predominately as cations, compared to 50% for the base case.

Among the 25 dissolved trace metals and 7 radioactive elements:

- As in the base case, about one-third of the trace metals and radionuclide elements are present predominantly as free (uncomplexed) cations (11 out of 32, or 34%). Downgrading the free Zn cation to the status of a secondary species is the only difference relative to the base case.
- A higher proportion are present as negatively-charged anions (13 out of 33, or 41%), compared to the base case (31%). The lists of species dominated by anionic oxyanions and hydroxides are identical to those for the base case, but the number dominated by anionic carbonate complexes increases from two (for the base case) to five for this bounding case due to the increased relative proportions of these complexes for Am, Ce, and Pu.
- None of the metal or radionuclide elements are dominated by cationic complexes, in contrast with the base case for which six of these elements (19% of 32) are in this category.
- The remaining eight elements are dominated by neutral species (24% of 33), compared to four elements (12%) for the base case. In addition to those listed for the base case (B, Hg, Cu, and Pb), the four elements added to this category are Be, Fe, Np, and Zn.

**Table 6-4. Dominant geochemical speciation for bounding case 3**

| Dissolved species | Neutral (uncharged) | Cation | Anion | Category[a] total |
|---|---|---|---|---|
| Free ion | — | Ba, Cd, Ca, Cs, Co, Li, Mg, Mn, Ni, K, Ag, Na, Ra, Sr, Tl, (Zn) | Br, Cl, F | *Primary:* 18<br>*Secondary:* 1 |
| Oxide species | — | — | Sb, As, Cr, Mo, N, P, Se, S, V, Tc | *Primary:* 10<br>*Secondary:* — |
| Hydroxide species | B, Be, Fe, Hg, Si | (Pb) | Al, (B), (Fe), Sn | *Primary:* 7<br>*Secondary:* 3 |
| Carbonate species | (Cd), (Co), Cu, (Ni), Np, Pb, (Pu), Zn | (Am) | Am, C, Ce, Pu, U | *Primary:* 9<br>*Secondary:* 5 |
| *Category[a] total* | *Primary:* 9<br>*Secondary:* 4 | *Primary:* 15<br>*Secondary:* 3 | *Primary:* 20<br>*Secondary:* 2 | *Primary:* 44<br>*Secondary:* 9 |

Source: Table B-4

[a] Primary species are those accounting for the largest proportion of the total elemental concentration. Elements shown in parentheses indicate species that are secondary in dominance but that account for more than 25% of the total elemental concentration.

Underlined species indicate differences relative to base case speciation.

Bounding case 4. Median concentrations in the regional aquifer, methanogenic conditions. The last two bounding cases are scoping calculations to identify the extent to which oxidation states and speciation might change under very reducing conditions. These calculations are subject to several caveats, assumptions, and limitations such as those briefly outlined in Section 7. Case-specific modeling would be necessary to obtain reliable modeling results.

Comparison of Table B-5 (this bounding case) to Table B-1 (base case) shows that, under methanogenic conditions, the dominant oxidation states of the following 13 elements (30% of 44) shifts to their reduced forms:

- Major elements: N, S

  Note: C is not listed here because only a negligible proportion of the C present as carbonate species may be reduced to methane.

- Trace metals: Sb, As, Cr, Cu, Fe, Se, U, V
- Radioelements: Np, Pu, Tc

Although the speciation calculations for this report are not set up to address the effects of mineral precipitation and dissolution, this aspect plays central role in determining elemental speciation and transport characteristics, particularly for trace metals and radionuclides, for groundwaters in which reducing conditions have developed. Based upon significant shifts in mineral saturation indices from undersaturation for oxic conditions to oversaturation under reducing (methanogenic or Fe-reducing conditions), modeling results support the hypothesis that elemental concentrations are likely to fall below detection levels for a large number of the trace metals in local groundwaters if reducing conditions develop. (Note, however, that it may be difficult to separate the effects of mineral precipitation from those of sorption when evaluating analytical data.) Table B-7 tabulates mineral phases which could conceivably remove aqueous species of 16 trace metals and 3 radioelements from solution:

- Metal hydroxide or oxide: Cr, Cu, Fe, U, V, Np, Tc
- Fe(II) or Cr(III) mixed metal oxide: Cd, Cr, Co, Cu, Fe, Ni
- Metal sulfide: As, Cd, Co, Cu, Fe, Pb, Hg, Mo, Ni, Ag, Zn
- Metal selenide: Sb, Cd, Cu, Fe, Pb, Hg, Mo, Ni, Se, Ag, Zn
- Phosphate: Pu
- Silicates or other phases: As, Fe, Ni, U

Excluded from the list above are mineral phases that are supersaturated to the same degree for the base case as for the methanogenic bounding case because it is assumed that precipitation of these mineral phases is not directly affected by redox conditions.

Conversely, the modeling results also support the hypothesis that some trace metals could increase in concentration due to dissolution of mineral phases if reducing environments develop in local groundwaters. Based upon significant shifts in mineral saturation indices from oversaturation for oxic conditions to undersaturation for reducing conditions, mineral dissolution could result in increased concentrations of the following 12 trace metals (Table B-7):

- Sb, As, Co, Cu, Fe, Pb, Mn, Mo, Ni, Sr, Zn, Ce

However, it may be difficult to separate contributions from dissolution versus desorption when evaluating analytical data for these effects.

An additional column has been added to the summary table for this bounding case (Table 6-5) to capture the possible effects of mineral precipitation. Altogether, 20 out of 44 elements (45%) could be removed from solution by mineral precipitation. This number includes 19 of the 32 trace metals and radionuclides (59%). In contrast, with the exception of S, the 8 major elements are not directly affected by reducing

conditions, and the following 7 elements are predicted to be unchanged from the base case with respect to oxidation state and dominant speciation:

- Major elements as free cations: Ca, Mg, K, Na
- Major elements as anions: Cl, C
- Major elements as neutral species: Si

Twenty-four trace elements are also predicted to be unchanged from the base case with respect to oxidation state and dominant speciation:

- Trace metals as free cations: Ba, Co, Cs, Cu, Fe, Li, Mn, Ni, Ra, Sr, Tl, Zn
- Trace metals and radionuclides as complexed cations: Am, Be, Ce, Pb
- Trace metals as neutral species: As, B, Sb
- Anions: Br, F, Al, Mo, Sn

Dominant speciation changes for three trace species: If not completely removed from solution through mineral precipitation, then As and Sb are present as neutral hydroxide complexes, and Fe as a bare cation.

**Table 6-5. Dominant geochemical speciation for bounding case 4**

| Dissolved species | Neutral (uncharged) | Cation | Anion | Precipitated as solid phase | Category[a] total |
|---|---|---|---|---|---|
| Free ion | — | Ba, Ca, Cs, Li, Mg, Mn, K, Na, Ra, Sr, Tl<br>Co[b], Cu[b], <u>Fe</u>[b], Ni[b], Zn[b] | Br, Cl, F | — | *Primary:* 19<br>*Secondary:* —<br>*Mineral phases:* — |
| Oxide species | (<u>Sb</u>[b]) | — | Mo[b] | Cd, Co, Cr, Cu, Fe, Ni, Np, Pu, Tc, U, V | *Primary:* 1<br>*Secondary:* 1<br>*Mineral phases:* 11 |
| Hydroxide species | <u>As</u>[b], B, (Be), <u>Sb</u>[b], Si | (<u>Am</u>), Be, Pb[b] | Al, Sn | — | *Primary:* 8<br>*Secondary:* 2<br>*Mineral phases:* — |
| Carbonate species | — | Am, Ce | C, (Ce) | — | *Primary:* 3<br>*Secondary:* 1<br>*Mineral phases:* — |
| Sulfide or selenide species | — | — | — | Ag, As, Cd, Co, Cu, Fe, Hg, Mo, Ni, Pb, S, Sb, Se, Zn | *Primary:* —<br>*Secondary:* —<br>*Mineral phases:* 14 |
| Phosphate species | — | — | — | (Pu) | *Primary:* —<br>*Secondary:* —<br>*Mineral phases:* — |
| Other species | — | <u>$NH_4^+$</u> | — | (U) | *Primary:* 1<br>*Secondary:* —<br>*Mineral phases:* — |
| *Category[a] total* | *Primary:* 4<br>*Secondary:* 2 | *Primary:* 21<br>*Secondary:* 1 | *Primary:* 7<br>*Secondary:* 1 | *Primary:* —<br>*Secondary:* —<br>*Mineral phases:* 20[c] | *Primary:* 32<br>*Secondary:* 4<br>*Mineral phases:* 20[c] |

Source: Tables B-5 and B-7

[a] Primary species are those accounting for the largest proportion of the total elemental concentration. Elements shown in parentheses indicate species that are secondary in dominance but that account for more than 25% of the total elemental concentration.

[b] This element is included both in the mineral phase category as well as in the aqueous species category because, under some reducing conditions, the effects of mineral dissolution or competition with other complexing aqueous species may exert a greater control on its aqueous concentration and speciation than does its removal from solution by mineral precipitation.

[c] Total sum of mineral phases excludes duplication of elements present in more than one mineral phase. However, it includes some elements that are listed both in the mineral phase category as well as in the aqueous species category. See footnote b.

<u>Underlined</u> aqueous species indicate differences relative to base case speciation

Bounding case 5. Median concentrations in the intermediate perched zone, methanogenic conditions. Table B-6 (this bounding case) is compared to Table B-5 (the methanogenic bounding case for the regional aquifer) to identify the extent to which outcomes may be affected by differences in elemental concentrations between the intermediate perched zone and the regional aquifer. As noted in the discussion of bounding case 2, median alkalinity in the intermediate perched zone (38.45 mg/L as $CaCO_3$) is only 58% of that in the regional aquifer (66 mg/L as $CaCO_3$), such that the significance of carbonate species should be somewhat diminished and that of other species should be more prominent. Nonetheless, the overall modeling outcome supports a tentative conclusion that, within the limitations of this modeling study, oxidation states and dominant speciation are probably very similar for these two methanogenic bounding cases.

**Table 6-6. Dominant geochemical speciation for bounding case 5**

| Dissolved species | Neutral (uncharged) | Cation | Anion | Precipitated as solid phase | Category[a] total |
|---|---|---|---|---|---|
| Free ion | — | Ba, Ca, Cs, Li, Mg, Mn, K, Na, Ra, Sr, Tl<br>Co[b], Cu[b], Fe[b], Ni[b], Zn[b] | Br, Cl, F | — | *Primary:* 19<br>*Secondary:* —<br>*Mineral phases:* — |
| Oxide species | (Sb[b]) | — | Mo[b] | Cd, Co, Cr, Cu, Fe, Ni, Np, Pu, Tc, U, V | *Primary:* 1<br>*Secondary:* 1<br>*Mineral phases:* 11 |
| Hydroxide species | As[b], B, (Be), Sb[b], Si | (Am), Be, Pb[b] | Al, Sn | — | *Primary:* 8<br>*Secondary:* 2<br>*Mineral phases:* — |
| Carbonate species | — | Am, Ce | C, (Ce) | — | *Primary:* 3<br>*Secondary:* 1<br>*Mineral phases:* — |
| Sulfide or selenide species | — | — | — | Ag, As, Cd, Co, Cu, Fe, Hg, Mo, Ni, Pb, S, Sb, Se, Zn | *Primary:* —<br>*Secondary:* —<br>*Mineral phases:* 14 |
| Phosphate species | — | — | — | (Pu) | *Primary:* —<br>*Secondary:* —<br>*Mineral phases:* — |
| Other species | — | $NH_4^+$ | — | (U) | *Primary:* 1<br>*Secondary:* —<br>*Mineral phases:* — |
| *Category[a] total* | *Primary:* 4<br>*Secondary:* 2 | *Primary:* 21<br>*Secondary:* 1 | *Primary:* 7<br>*Secondary:* 1 | *Primary:* —<br>*Secondary:* —<br>*Mineral phases:* 20[c] | *Primary:* 32<br>*Secondary:* 4<br>*Mineral phases:* 20[c] |

Source: Tables B-6 and B-7

[a] Primary species are those accounting for the largest proportion of the total elemental concentration. Elements shown in parentheses indicate species that are secondary in dominance but that account for more than 25% of the total elemental concentration.

[b] This element is included both in the mineral phase category as well as in the aqueous species category because, under some reducing conditions, the effects of mineral dissolution or competition with other complexing aqueous species may exert a greater control on its aqueous concentration and speciation than does its removal from solution by mineral precipitation.

[c] Total sum of mineral phases excludes duplication of elements present in more than one mineral phase. However, it includes some elements that are listed both in the mineral phase category as well as in the aqueous species category. See footnote b.

Underlined aqueous species indicate differences relative to base case speciation

## 7. LIMITATIONS

The modeling described in this report has several limitations, such that its results should not be used out of context. These model calculations cannot take the place of case-specific modeling that is tailored to the specific issues to be addressed:

- The computer program was run solely for the purpose of calculating the dominant speciation for fixed elemental concentrations, e.g., the solution was not allowed to add or remove elements to approach equilibrium with mineral phases.

- Similarly, the model runs do not simulate changes in elemental concentrations due to adsorption or desorption from mineral surfaces.

- Analyses below the method detection limit as well as below the contract-required reporting limit are included in the background groundwater statistics, potentially biasing median and upper limit values. This is particularly an issue of which to be aware for elements that have high nondetect rates, as is the case for several trace elements, for example Sb, Be, Tl, and Cd.

- Water-quality data for filtered samples used to establish background groundwater compositions presumably include contributions from colloids for some species, thereby potentially biasing median and upper limit values.

- Dissolved organic carbon was not included in the model simulation although this component complexes strongly with some cationic species.

- The effects of microbial activity on modifying oxidation states and speciation are not addressed by the model. Many trace species can be reduced or oxidized by microbes, in a direction counter to the reaction path predicted based on thermodynamic calculations. For this and many other reasons, traditional geochemical equilibrium models are generally poor predictors of redox conditions in natural groundwater systems.

- The set of bounding cases probably adequately bound changes in dominant oxidation state for the species considered, but not the possible variability in dominant speciation. This limitation is due to a number of reasons, including the large number of permutations possible for elemental concentrations. In particular, the dominant speciation for several metals and radioactive elements are extremely sensitive to ligand concentrations ($HCO_3^-$, $CO_3^{2-}$, $PO_4^{3-}$, and $F^-$).

- The available thermodynamic databases sometimes yield significantly different outcomes for the dominant speciation of selected elements or for mineral saturation indices.

- The calculated mineral saturation indices (discussed under the methanogenic bounding cases) do not take into account kinetic effects or competition between species in mineral dissolution and precipitation. For example, dissolved sulfide is assumed to be equally available to all trace metals that form sulfide mineral phases, although in reality the sulfide would probably be completely sequestered by just one or two of those metals.

## 8. SUMMARY

Based upon the modeling results presented in this report, the following tables summarize the dominant oxidation states and speciation of inorganic dissolved species calculated for local groundwater, under oxic conditions. The far-right column notes conditions under which the calculated oxidation state or speciation may not be valid.

**Table 8-1. General Inorganic Analytes**

| Analyte | Possible Oxidation States of Aqueous Species in Groundwater[a] | Dominant Oxidation State of Aqueous Species in the Regional Aquifer | Dominant Aqueous Species in the Regional Aquifer[b] | Geochemical conditions identified by bounding cases as having the potential to cause a significant shift in dominant speciation |
|---|---|---|---|---|
| Alkalinity | C(-4, +4) | C(+4) | $HCO_3^-$ | None |
| Bromide | Br(-1) | Br(-1) | $Br^-$ | None |
| Calcium | Ca(+2) | Ca(+2) | $Ca^{2+}$ | None |
| Chloride | Cl(-1) | Cl(-1) | $Cl^-$ | None |
| Fluoride | F(-1) | F(-1) | $F^-$ | None |
| Magnesium | Mg(+2) | Mg(+2) | $Mg^{2+}$ | None |
| Nitrogen | N(0,+3,+5) | N(+5) | $NO_3^-$ | Reducing conditions |
| Phosphorus | P(+5) | P(+5) | $HPO_4^{2-}$, $H_2PO_4^-$ | None |
| Potassium | K(+1) | K(+1) | $K^+$ | None |
| Silicon | Si(+4) | Si(+4) | $H_4SiO_4$ | None |
| Sodium | Na(+1) | Na(+1) | $Na^+$ | None |
| Sulfate | S(+6) | S(+6) | $SO_4^{2-}$ | Reducing conditions |

[a] "Possible oxidation states" are those which could account for at least 10% of the total dissolved concentration within the range of Eh, pH, and alkalinity concentrations that constitute background conditions.

[b] Listed species are in order of relative concentration for all species that constitute at least 10% of the total concentration for base case conditions in the regional aquifer (median concentrations, pH, and alkalinity, Eh = 533 mV, pE = 9.0); i.e., if only one species is listed, then it alone accounts for more than 90% of the total concentration of that analyte.

**Table 8-2. Metal Analytes**

| Analyte | Possible Oxidation States of Aqueous Species in Groundwater[a] | Dominant Oxidation State in the Regional Aquifer | Dominant Dissolved Species in the Regional Aquifer[b] | Geochemical conditions identified by bounding cases as having the potential to cause a significant shift in dominant speciation |
|---|---|---|---|---|
| Aluminum | +3 | +3 | $Al(OH)_4^-$ | None |
| Antimony | +3, +5 | +5 | $SbO_3^-$ | Reducing conditions |
| Arsenic | +3, +5 | +5 | $[HAsO_4]^{2-}$, $H_2AsO_4^-$ | Reducing conditions |
| Barium | +2 | +2 | $Ba^{+2}$ | None |
| Beryllium | +2 | +2 | $BeOH^+$, $Be(OH)_2$ | Elevated pH/Alkalinity |
| Boron | +3 | +3 | $H_3BO_3$ | None |
| Cadmium | +2 | +2 | $Cd^{+2}$ | Reducing conditions |
| Chromium | +3, +6 | +6 | $CrO_4^{2-}$ | Reducing conditions |
| Cobalt | +2 | +2 | $Co^{2+}$ | Reducing conditions |
| Copper | +1, +2 | +2 | $CuCO_3$, $CuOH^+$ | Reducing conditions |
| Iron | +2, +3 | +3 | $Fe(OH)_2^+$, $Fe(OH)_3$ | Elevated pH/Alkalinity<br>Reducing conditions |
| Lead | +2 | +2 | $PbCO_3$, $PbOH^+$, $Pb^{2+}$ | Reducing conditions |
| Lithium | +1 | +1 | $Li^+$ | None |
| Manganese | +2, +3, +6, +7 | +2 | $Mn^{2+}$ | Reducing conditions |
| Mercury | 0, +2 | +2 | $Hg(OH)_2$ | Reducing conditions |
| Molybdenum | +6 | +6 | $MoO_4^{2-}$ | Reducing conditions |
| Nickel | +2 | +2 | $Ni^{2+}$, $NiHCO_3^-$, $NiCO_3$ | Elevated pH/Alkalinity<br>Reducing conditions |
| Selenium | -2, +4, +6 | +6 | $SeO_4^{2-}$ | Reducing conditions |
| Silver | +1 | +1 | $Ag^+$ | Reducing conditions |
| Strontium | +2 | +2 | $Sr^{2+}$ | None |
| Thallium | +1, +3 | +1 | $Tl^+$ | None |
| Tin | +4 | +4 | $Sn(OH)_6^{-2}$ | None |
| Uranium | +4, +5, +6 | +6 | $[UO_2(CO_3)_2]^{2-}$, $[UO_2(CO_3)_3]^{4-}$ | Elevated pH/Alkalinity<br>Reducing conditions |
| Vanadium | +3, +4, +5 | +5 | $H_2VO_4^-$, $HVO_4^{2-}$ | Reducing conditions |
| Zinc | +2 | +2 | $Zn^{2+}$, $ZnCO_3$ | Elevated pH/Alkalinity<br>Reducing conditions |

[a] "Possible oxidation states" are those which could account for at least 10% of the total dissolved concentration within the range of Eh, pH, and alkalinity concentrations that constitute background conditions.

[b] Listed species are in order of relative concentration for all species that constitute at least 10% of the total concentration for base case conditions in the regional aquifer (median concentrations, pH, and alkalinity, Eh = 533 mV, pE = 9.0); i.e., if only one species is listed, then it alone accounts for more than 90% of the total concentration of that analyte.

**Table 8-3. Radioelements**

| Analyte with radioactive isotopes | Possible Oxidation States of Aqueous Species in Groundwater[a] | Dominant Oxidation State in the Regional Aquifer | Dominant Aqueous Species in the Regional Aquifer[b] | Geochemical conditions identified by bounding cases as having the potential to cause a significant shift in dominant speciation |
|---|---|---|---|---|
| Americium (e.g., Am-241) | +3 | +3 | $AmCO_3^+$, $Am(OH)_2^+$, $Am(OH)^{2+}$ | Elevated pH/Alkalinity |
| Cerium (e.g., Ce139, 141, 144) | +3 | +3 | $CeCO_3^+$, $Ce(CO_3)^{2-}$ | Elevated pH/Alkalinity |
| Cesium (e.g., Cs-137) | +1 | +1 | $Cs^+$ | None |
| Cobalt[c] (e.g., Co-60) | +2 | +2 | $Co^{2+}$ | Reducing conditions |
| Europium[d] (e.g., Eu-152, Eu-154, Eu-155) | +3 | +3 | $EuCO_3^+$, $Eu(CO_3)^{2-}$ | Elevated pH/Alkalinity |
| Lanthanum[d] (e.g. La-140) | +3 | +3 | $LaCO_3^+$, $La(CO_3)^{2-}$ | Elevated pH/Alkalinity |
| Neodymium[d] (e.g. Nd-147) | +3 | +3 | $NdCO_3^+$, $Nd(CO_3)^{2-}$ | Elevated pH/Alkalinity |
| Neptunium (e.g, Np-237) | +4, +5 | +5 | $NpO_2^+$, $NpO_2CO_3^-$ | Reducing conditions |
| Plutonium (e.g., Pu-238, Pu-239, Pu-240) | +3, +4, +5, +6 | +5, +6 | $PuO_2^+$, $PuO_2CO_3^-$, $PuO_2CO_3$ | Elevated pH/Alkalinity<br>Reducing conditions |
| Radium (e.g., Ra-226, Ra-228) | +2 | +2 | $Ra^{2+}$ | None |
| Strontium[c] (e.g., Sr-90) | +2 | +2 | $Sr^{2+}$ | None |
| Technetium (e.g., Tc-99) | +4, +6, +7 | +7 | $TcO_4^-$ | Reducing conditions |
| Tritium | +1 | +1 | $HTO^0$ | None |
| Uranium[c] (e.g., U-234, U-235, U-236, U-238) | +4, +5, +6 | +6 | $[UO_2(CO_3)_2]^{2-}$, $[UO_2(CO_3)_3]^{4-}$ | Elevated pH/Alkalinity<br>Reducing conditions |

[a] "Possible oxidation states" are those which could account for at least 10% of the total dissolved concentration within the range of Eh, pH, and alkalinity concentrations that constitute background conditions.

[b] Listed species are in order of relative concentration for all species that constitute at least 10% of the total concentration for base case conditions in the regional aquifer (median concentrations, pH, and alkalinity, Eh = 530 mV, pE = 9.0); i.e., if only one species is listed, then it alone accounts for more than 90% of the total concentration of that analyte.

[c] Oxidation state and speciation are based on that shown for this element in Table 8-2.

[d] None of the available thermodynamic databases contains data for these lanthanide elements. Hence, their dominant oxidation states and species are assumed to be analogous to those calculated for another member of the lanthanide series, cerium.

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# Appendix A

## Range and Median Values of Dissolved Species in Background Groundwater

Table A-1. Median and Upper Limits for Concentrations of Dissolved Species in the Regional Aquifer

| Analyte (sorted alphabetically by name) | Symbol | Units | % Non-detects | Median Value | Upper Limit[a] | |
|---|---|---|---|---|---|---|
| Alkalinity (total carbonate) | $CaCO_3$ | mg/L | 0 | 66 | 105.1 | UTL |
| Aluminum | Al | µg/L | 85 | 34 | 73.5 | Maximum |
| Ammonia | $NH_3$-N | mg/L | 93 | ND[b] (<0.01) | 0.05 | Max detected[c] |
| Antimony | Sb | µg/L | 98 | 0.25 | 1.00 | Maximum |
| Arsenic | As | µg/L | 77 | 3.00 | 16.3 | Maximum |
| Barium | Ba | µg/L | 5 | 20.8 | 69.2 | UTL |
| Beryllium | Be | µg/L | 100 | 0.24 | 0.50 | Maximum |
| Boron | B | µg/L | 29 | 13.65 | 86.1 | Maximum |
| Bromide | Br | mg/L | 47 | 0.03 | 0.22 | Maximum |
| Cadmium | Cd | µg/L | 97 | 0.05 | 0.50 | Maximum |
| Calcium | Ca | mg/L | 0 | 11.7 | 24.12 | UTL |
| Chloride | Cl | mg/L | 0 | 2.22 | 3.75 | UTL |
| Chromium | Cr | µg/L | 20 | 3.47 | 6.62 | UTL |
| Cobalt | Co | µg/L | 89 | 0.50 | 7.00 | Maximum |
| Copper | Cu | µg/L | 87 | 1.50 | 62.2 | Maximum |
| Fluoride | F | mg/L | 9 | 0.32 | 0.53 | UTL |
| Iron | Fe | µg/L | 71 | ND (9.00) | 102 | 90th percentile[d] |
| Lead | Pb | µg/L | 82 | 0.25 | 4.60 | Maximum |
| Lithium | Li | µg/L | 0 | 23.0 | 32.16 | UTL |
| Magnesium | Mg | mg/L | 0 | 2.96 | 4.81 | UTL |
| Manganese | Mn | µg/L | 67 | ND (1.00) | 16 | Max detected[c] |
| Mercury | Hg | µg/L | 97 | 0.03 | 0.26 | Maximum |
| Molybdenum | Mo | µg/L | 49 | 1.09 | 3.82 | UTL |
| Nickel | Ni | µg/L | 78 | ND (0.50) | 1.7 | Max detected |
| Nitrate (as N) | $NO_3$-N | mg/L | 9 | 0.33 | 0.75 | UTL |
| pH | pH | SU | 0 | 7.82 | 8.65 | UTL |
| Potassium | K | mg/L | 0 | 1.89 | 3.14 | UTL |
| Selenium | Se | µg/L | 99 | 1.25 | 4.60 | Maximum |
| Silicon dioxide | SiO2 | mg/L | 2 | 69.55 | 98.98 | UTL |
| Silver | Ag | µg/L | 100 | 0.42 | 2.50 | Maximum |
| Sodium | Na | mg/L | 0 | 12.5 | 28.55 | UTL |
| Strontium | Sr | µg/L | 0 | 55.55 | 179.8 | UTL |
| Sulfate | $SO_4$ | mg/L | 3 | 2.9 | 6.22 | UTL |
| Thallium | Tl | µg/L | 82 | 0.20 | 0.83 | Maximum |
| Tin | Sn | µg/L | 99 | ND (1.25) | 3.60 | Maximum |
| Titanium | Ti | µg/L | 100 | ND (0.50) | 1.00 | MDL |
| Total Phosphate (as P) | $PO_4$-P | mg/L | 69 | ND (0.02) | 0.34 | Max detected |
| Uranium | U | µg/L | 3 | 0.45 | 1.52 | UTL |

| Analyte (sorted alphabetically by name) | Symbol | Units | % Non-detects | Median Value | Upper Limit [a] | |
|---|---|---|---|---|---|---|
| Vanadium | V | µg/L | 6 | 7.90 | 25.58 | UTL |
| Zinc | Zn | µg/L | 61 | 1.92 | 41.1 | Max detected[c] |

Source of values: Table 4.2-3 in Groundwater Background Investigation Report, Rev. 2 (LANL 2007, 094856)

[a] Except as noted otherwise, the upper limit is set at the upper threshold limit (UTL) if available, the 90th percentile for filtered samples (if available), or the maximum detected values for the background data set.

[b] ND = Not detected.

[c] The upper limits for ammonia, manganese, and zinc are set at the maximum concentrations detected in background samples collected only from wells because the range in concentrations in background samples collected from springs that discharge from the regional aquifer extend significantly outside the range of values observed in the well samples.

[d] The upper limit for dissolved iron is set at the 90th percentile for total (nonfiltered) iron. Percentiles were not calculated for dissolved iron due to the high proportion of nondetects in this dataset.

Table A-2. Background Values for Dissolved Species in the Intermediate Perched Zone

| Analyte (sorted alphabetically by name) | Symbol | Units | % Non-detects | Median Value | Upper Limit[a] | |
|---|---|---|---|---|---|---|
| Alkalinity (carbonate) | $CaCO_3$ | mg/L | 0 | 38.45 | 52.00 | UTL |
| Aluminum | Al | µg/L | 0 | 30.5 | 1066 | UTL |
| Ammonia | $NH_3$-N | mg/L | —[d] | — | [e] | — |
| Antimony | Sb | µg/L | 100 | ND (0.50) | 0.50 | Maximum |
| Arsenic | As | µg/L | 9 | 0.50 | 4.32 | UTL |
| Barium | Ba | µg/L | 0 | 15.5 | 71.83 | UTL |
| Beryllium | Be | µg/L | 100 | ND (0.50) | 0.50 | Maximum |
| Boron | B | µg/L | 0 | 8.25 | 15.12 | UTL |
| Bromide | Br | mg/L | 10 | 0.02 | 0.03 | UTL |
| Cadmium | Cd | µg/L | 100 | ND (0.50) | 0.50 | Maximum |
| Calcium | Ca | mg/L | 0 | 7.5 | 17.31 | UTL |
| Chloride | Cl | mg/L | 0 | 1.37 | 8.37 | UTL |
| Chromium | Cr | µg/L | 77 | ND (0.50) | 2.40 | Maximum |
| Cobalt | Co | µg/L | 95 | ND (0.50) | 1.20 | Maximum |
| Copper | Cu | µg/L | 32 | 1.37 | 5.32 | UTL |
| Fluoride | F | mg/L | 0 | 0.12 | 0.23 | UTL |
| Iron | Fe | µg/L | 45 | 20.00 | 102[e] | — |
| Lead | Pb | µg/L | 86 | 0.10 | 0.30 | Maximum |
| Lithium | Li | µg/L | 0 | 7.90 | 61.25 | UTL |
| Magnesium | Mg | mg/L | 0 | 1.65 | 6.12 | UTL |
| Manganese | Mn | µg/L | 77 | ND (0.50) | 3.63 | Maximum |
| Mercury | Hg | µg/L | 100 | ND (0.03) | 0.03 | Maximum |
| Molybdenum | Mo | µg/L | 55 | ND (0.50) | 4.30 | Maximum |
| Nickel | Ni | µg/L | 86 | ND (0.50) | 29.00 | Maximum |
| Nitrate (as N) | $NO_3$-N | mg/L | 0 | 0.34 | 2.65 | UTL |
| pH | pH | SU | 0 | 7.39 | 8.80 | UTL |
| Phosphate (as P) | $PO_4$-P | mg/L | 14 | 0.02 | 0.08 | UTL |
| Potassium | K | mg/L | 0 | 1.82 | 10.03 | UTL |
| Selenium | Se | µg/L | 100 | ND (0.50) | 1.25 | Maximum |
| Silicon dioxide | SiO2 | mg/L | 0 | 24.35 | 50.72 | UTL |
| Silver | Ag | µg/L | 100 | ND (0.50) | 0.50 | Maximum |
| Sodium | Na | mg/L | 0 | 7.23 | 12.19 | UTL |
| Strontium | Sr | µg/L | 0 | 55 | 154.76 | UTL |
| Sulfate | $SO_4$ | mg/L | 0 | 4.08 | 4.48 | 95th percentile |
| Thallium | Tl | µg/L | 100 | ND (0.50) | 0.50 | Maximum |
| Tin | Sn | µg/L | 100 | ND (0.50) | 0.50 | Maximum |
| Titanium | Ti | µg/L | 50 | 0.75 | 8.96 | UTL |
| Uranium | U | µg/L | 43 | 0.30 | 0.72 | UTL |

| Analyte (sorted alphabetically by name) | Symbol | Units | % Non-detects | Median Value | Upper Limit[a] | |
|---|---|---|---|---|---|---|
| Vanadium | V | µg/L | 23 | 2.40 | 4.91 | UTL |
| Zinc | Zn | µg/L | 59 | ND (0.75) | 19.00 | Maximum |

Source of values: Table 4.2-2 in Groundwater Background Investigation Report, Rev. 2 (LANL 2007, 094856).

[a] Except as noted otherwise, the upper limit is set at the upper threshold limit (UTL) if available, the 90th percentile for filtered samples (if available), or the maximum detected values for the background data set.

[b] ND = Not detected.

[c] The upper limits for ammonia, manganese, and zinc are set at the maximum concentrations detected in background samples collected only from wells because the range in concentrations in background samples collected from springs that discharge from the regional aquifer extend significantly outside the range of values observed in the well samples.

[d] The upper limit for dissolved iron is set at the 90th percentile for total (nonfiltered) iron. Percentiles were not calculated for dissolved iron due to the high proportion of nondetects in this dataset.

[e] Insufficient data to calculate statistical distribution parameters; use same limits as for regional aquifer (Table A-1).

# Appendix B

## Summary tables of oxidation states and geochemical speciation for six modeling cases

Table B-1. Geochemical Speciation for Base Case: Regional Aquifer, Median Concentrations

| Analyte (sorted alphabetically by name) | Dominant oxidation state | Dominant species (Percent of total) | | |
|---|---|---|---|---|
| | | 75-100% | 25-75% | 10-25% |
| Alkalinity (carbonate) | C(+4) | HCO3- | — | — |
| Aluminum | Al(+3) | Al(OH)4- | — | — |
| Antimony | Sb(+5) | SbO3- | — | — |
| Arsenic | As(+5) | HAsO4-2 | — | H2AsO4- |
| Barium | Ba(+2) | Ba+2 | — | — |
| Beryllium | Be(+2) | — | BeOH+, Be(OH)2 | — |
| Boron | B(+3) | H3BO3 | — | — |
| Bromide | Br(-1) | Br- | — | — |
| Cadmium | Cd(+2) | Cd+2 | — | — |
| Calcium | Ca(+2) | Ca+2 | — | — |
| Chloride | Cl(-1) | Cl- | — | — |
| Chromium | Cr(+6) | CrO4-2 | — | — |
| Cobalt | Co(+2) | Co+2 | — | — |
| Copper | Cu(+2) | CuCO3 | — | CuOH+ |
| Fluoride | F(-1) | F- | — | — |
| Iron | Fe(+3) | — | Fe(OH)2+, Fe(OH)3 | — |
| Lead | Pb(+2) | PbCO3 | — | PbOH+, Pb+2 |
| Lithium | Li(+1) | Li+ | — | — |
| Magnesium | Mg(+2) | Mg+2 | — | — |
| Manganese | Mn(+2) | Mn+2 | — | — |
| Mercury | Hg(+2) | Hg(OH)2 | — | — |
| Molybdenum | Mo(+6) | MoO4-2 | — | — |
| Nickel | Ni(+2) | Ni+2 | — | NiHCO3+, NiCO3 |
| Nitrogen | N(+5) | NO3- | — | — |
| Phosphorus | P(+5) | HPO4-2 | — | H2PO4- |
| Potassium | K(+1) | K+ | — | — |
| Selenium | Se(+6) | SeO4-2 | — | — |
| Silica | Si(+4) | H4SiO4 | — | — |
| Silver | Ag(+1) | Ag+ | — | AgCl |
| Sodium | Na(+1) | Na+ | — | — |
| Strontium | Sr(+2) | Sr+2 | — | — |
| Sulfate | S(+6) | SO4-2 | — | — |
| Thallium | Tl(+1) | Tl+ | — | — |
| Tin | Sn(+4) | Sn(OH)6-2 | — | — |
| Uranium | U(+6) | — | UO2(CO3)2-2 | UO2(CO3)3-4 |
| Vanadium | V(+5) | H2VO4- | — | HVO4-2 |
| Zinc | Zn(+2) | Zn+2 | — | ZnCO3 |

| Analyte (sorted alphabetically by name) | Dominant oxidation state | Dominant species (Percent of total) | | |
|---|---|---|---|---|
| | | 75-100% | 25-75% | 10-25% |
| Radioactive elements (speciation calculated using PHREEQCdata025.dat) | | | | |
| Americium | Am(+3) | — | AmCO3+ | Am(OH)2+, AmOH+2 |
| Cerium | Ce(+3) | — | CeCO3+, Ce(CO3)2- | — |
| Cesium | Cs(+1) | Cs+ | — | — |
| Neptunium | Np(+5) | | NpO2+, NpO2CO3-, | |
| Plutonium | Pu(+5, +6) | — | PuO2+, PuO2CO3- | PuO2CO3 |
| Radium | Ra(+2) | Ra+2 | — | — |
| Technetium | Tc(+7) | TcO4- | — | — |

Data base: Minteq.v4.dat (except as noted)

Table B-2. Geochemical speciation for Bounding Case 1: Regional Aquifer, UTL Concentrations

| Analyte (sorted alphabetically by name) | Dominant oxidation state | Dominant species (Percent of total) | | |
|---|---|---|---|---|
| | | 75-100% | 25-75% | 10-25% |
| Alkalinity (carbonate) | C(+4) | HCO3- | — | — |
| Aluminum | Al(+3) | Al(OH)4- | — | — |
| Antimony | Sb(+5) | SbO3- | — | — |
| Arsenic | As(+5) | HAsO4-2 | — | — |
| Barium | Ba(+2) | Ba+2 | — | — |
| Beryllium | Be(+2) | Be(OH)2 | BeOH+ | — |
| Boron | B(+3) | H3BO3 | — | — |
| Bromide | Br(-1) | Br- | — | — |
| Cadmium | Cd(+2) | — | Cd+2, CdCO3 | — |
| Calcium | Ca(+2) | Ca+2 | — | — |
| Chloride | Cl(-1) | Cl- | — | — |
| Chromium | Cr(+6) | CrO4-2 | — | — |
| Cobalt | Co(+2) | — | Co+2, CoCO3 | — |
| Copper | Cu(+2) | CuCO3 | — | Cu(CO3)2-2 |
| Fluoride | F(-1) | F- | — | — |
| Iron | Fe(+3) | — | Fe(OH)3, Fe(OH)4- | Fe(OH)2+ |
| Lead | Pb(+2) | PbCO3 | — | Pb(CO3)-2 |
| Lithium | Li(+1) | Li+ | — | — |
| Magnesium | Mg(+2) | Mg+2 | — | — |
| Manganese | Mn(+2) | Mn+2 | — | — |
| Mercury | Hg(+2) | Hg(OH)2 | — | — |
| Molybdenum | Mo(+6) | MoO4-2 | — | — |
| Nickel | Ni(+2) | — | NiCO3, Ni+2 | — |
| Nitrogen | N(+5) | NO3- | — | — |
| Phosphorus | P(+5) | HPO4-2 | — | H2PO4- |
| Potassium | K(+1) | K+ | — | — |
| Selenium | Se(+6) | SeO4-2 | — | — |
| Silica | Si(+4) | H4SiO4 | — | — |
| Silver | Ag(+1) | Ag+ | — | AgCl |
| Sodium | Na(+1) | Na+ | — | — |
| Strontium | Sr(+2) | Sr+2 | — | — |
| Sulfate | S(+6) | SO4-2 | — | — |
| Thallium | Tl(+1) | Tl+ | — | — |
| Tin | Sn(+4) | Sn(OH)6-2 | — | — |
| Uranium | U(+6) | UO2(CO3)3-4 | — | UO2(CO3)2-2 |
| Vanadium | V(+5) | — | HVO4-2, H2VO4- | — |
| Zinc | Zn(+2) | — | ZnCO3, Zn+2 | ZnOH+ |

| Analyte (sorted alphabetically by name) | Dominant oxidation state | Dominant species (Percent of total) | | |
|---|---|---|---|---|
| | | 75-100% | 25-75% | 10-25% |
| Radioactive elements (speciation calculated using PHREEQCdata025.dat) | | | | |
| Americium | Am(+3) | — | Am(CO3)2-, AmCO3+, Am(OH)2+ | — |
| Cerium | Ce(+3) | Ce(CO3)2- | — | CeCO3+ |
| Cesium | Cs(+1) | Cs+1 | — | — |
| Neptunium | Np(+5) | — | NpO2CO3-, NpO2+ | — |
| Plutonium | Pu(+5, +6) | — | PuO2CO3-, PuO2CO3, PuO2+ | — |
| Radium | Ra(+2) | Ra+2 | — | — |
| Technetium | Tc(+7) | TcO4- | — | — |

Highlighted cells indicate differences from base case oxidation state or speciation

Table B-3. Geochemical Speciation for Bounding Case 2: Intermediate Perched Zones, Median Concentrations

| Analyte (sorted alphabetically by name) | Dominant oxidation state | Dominant species (Percent of total) | | |
|---|---|---|---|---|
| | | 75-100% | 25-75% | 10-25% |
| Alkalinity (carbonate) | C(+4) | HCO3- | — | — |
| Aluminum | Al(+3) | Al(OH)4- | — | — |
| Antimony | Sb(+5) | SbO3- | — | — |
| Arsenic | As(+5) | HAsO4-2 | — | H2AsO4- |
| Barium | Ba(+2) | Ba+2 | — | — |
| Beryllium | Be(+2) | BeOH+ | — | Be(OH)2 |
| Boron | B(+3) | H3BO3 | — | — |
| Bromide | Br(-1) | Br- | — | — |
| Cadmium | Cd(+2) | Cd+2 | — | — |
| Calcium | Ca(+2) | Ca+2 | — | — |
| Chloride | Cl(-1) | Cl- | — | — |
| Chromium | Cr(+6) | CrO4-2 | — | HCrO4- |
| Cobalt | Co(+2) | Co+2 | — | — |
| Copper | Cu(+2) | — | CuCO3 | Cu+2, CuOH+ |
| Fluoride | F(-1) | F- | — | — |
| Iron | Fe(+3) | Fe(OH)2+ | — | Fe(OH)3 |
| Lead | Pb(+2) | — | PbCO3 | Pb+2, PbOH+, PbHCO3+ |
| Lithium | Li(+1) | Li+ | — | — |
| Magnesium | Mg(+2) | Mg+2 | — | — |
| Manganese | Mn(+2) | Mn+2 | — | — |
| Mercury | Hg(+2) | Hg(OH)2 | — | — |
| Molybdenum | Mo(+6) | MoO4-2 | — | — |
| Nickel | Ni(+2) | Ni+2 | — | — |
| Nitrogen | N(+5) | NO3- | — | — |
| Phosphorus | P(+5) | — | HPO4-2, H2PO4- | — |
| Potassium | K(+1) | K+ | — | — |
| Selenium | Se(+6) | SeO4-2 | — | — |
| Silica | Si(+4) | H4SiO4 | — | — |
| Silver | Ag(+1) | Ag+ | — | — |
| Sodium | Na(+1) | Na+ | — | — |
| Strontium | Sr(+2) | Sr+2 | — | — |
| Sulfate | S(+6) | SO4-2 | — | — |
| Thallium | Tl(+1) | Tl+ | — | — |
| Tin | Sn(+4) | Sn(OH)6-2 | — | — |
| Uranium | U(+6) | UO2(HPO4)2-2 | — | UO2(CO3)2-2 |
| Vanadium | V(+5) | H2VO4- | — | — |
| Zinc | Zn(+2) | Zn+2 | — | — |

| Analyte (sorted alphabetically by name) | Dominant oxidation state | Dominant species (Percent of total) | | |
|---|---|---|---|---|
| | | 75-100% | 25-75% | 10-25% |
| Radioactive elements (speciation calculated using PHREEQCdata025.dat) | | | | |
| Americium | Am(+3) | — | AmCO3+ | AmOH+2 |
| Cerium | Ce(+3) | CeCO3+ | — | Ce(CO3)2- |
| Cesium | Cs(+1) | Cs+ | — | — |
| Neptunium | Np(+5) | NpO2+ | — | — |
| Plutonium | Pu(+5) | PuO2+ | — | PuO2CO3- |
| Radium | Ra(+2) | Ra+2 | — | — |
| Technetium | Tc(+7) | TcO4- | — | — |

Data base: Minteq.v4.dat (except as noted)

Table B-4. Geochemical Speciation for Bounding Case 3: Intermediate Perched Zones, UTL Concentrations

| Analyte (sorted alphabetically by name) | Dominant oxidation state | Dominant species (Percent of total) | | |
|---|---|---|---|---|
| | | 75-100% | 25-75% | 10-25% |
| Alkalinity (carbonate) | C(+4) | HCO3- | — | — |
| Aluminum | Al(+3) | Al(OH)4- | — | — |
| Antimony | Sb(+5) | SbO3- | — | — |
| Arsenic | As(+5) | HAsO4-2 | — | — |
| Barium | Ba(+2) | Ba+2 | — | — |
| Beryllium | Be(+2) | — | Be(OH)2 | BeOH+, Be(OH)3- |
| Boron | B(+3) | — | H3BO3, H2BO3- | — |
| Bromide | Br(-1) | Br- | — | — |
| Cadmium | Cd(+2) | — | Cd+2, CdCO3 | — |
| Calcium | Ca(+2) | Ca+2 | — | — |
| Chloride | Cl(-1) | Cl- | — | — |
| Chromium | Cr(+6) | CrO4-2 | — | — |
| Cobalt | Co(+2) | — | Co+2, CoCO3 | — |
| Copper | Cu(+2) | CuCO3 | — | Cu(OH)2, CuOH+ |
| Fluoride | F(-1) | F- | — | — |
| Iron | Fe(+3) | — | Fe(OH)3, Fe(OH)4- | — |
| Lead | Pb(+2) | — | PbCO3, PbOH+ | — |
| Lithium | Li(+1) | Li+ | — | — |
| Magnesium | Mg(+2) | Mg+2 | — | — |
| Manganese | Mn(+2) | Mn+2 | — | — |
| Mercury | Hg(+2) | Hg(OH)2 | — | — |
| Molybdenum | Mo(+6) | MoO4-2 | — | — |
| Nickel | Ni(+2) | — | Ni+2, NiCO3 | — |
| Nitrogen | N(+5) | NO3- | — | — |
| Phosphorus | P(+5) | — | HPO4-2, CaPO4- | — |
| Potassium | K(+1) | K+ | — | — |
| Selenium | Se(+6) | SeO4-2 | — | — |
| Silica | Si(+4) | H4SiO4 | — | — |
| Silver | Ag(+1) | Ag+ | — | AgCl |
| Sodium | Na(+1) | Na+ | — | — |
| Strontium | Sr(+2) | Sr+2 | — | — |
| Sulfate | S(+6) | SO4-2 | — | — |
| Thallium | Tl(+1) | Tl+ | — | — |
| Tin | Sn(+4) | Sn(OH)6-2 | — | — |
| Uranium | U(+6) | — | UO2(CO3)3-4, UO2(CO3)2-2 | — |
| Vanadium | V(+5) | — | HVO4-2, H2VO4- | — |
| Zinc | Zn(+2) | — | ZnCO3, Zn+2 | ZnOH+, Zn(OH)2 |

| Analyte (sorted alphabetically by name) | Dominant oxidation state | Dominant species (Percent of total) | | |
|---|---|---|---|---|
| | | 75-100% | 25-75% | 10-25% |
| Radioactive elements (speciation calculated using PHREEQCdata025.dat) | | | | |
| Americium | Am(+3) | — | Am(CO3)2-, AmCO3+, Am(OH)2+ | — |
| Cerium | Ce(+3) | Ce(CO3)2- | — | CeCO3+ |
| Cesium | Cs(+1) | Cs+ | — | — |
| Neptunium | Np(+5) | NpO2CO3 | — | NpO2+ |
| Plutonium | Pu(+5, +6) | — | PuO2CO3-, PuO2CO3 | — |
| Radium | Ra(+2) | Ra+2 | — | — |
| Technetium | Tc(+7) | TcO4- | — | — |

Data base: Minteq.v4.dat (except as noted)

Table B-5. Geochemical speciation for Bounding Case 4: Regional Aquifer, Methanogenic Conditions

| Analyte (sorted alphabetically by name) | Dominant oxidation state | Dominant species (Percent of total) | | |
|---|---|---|---|---|
| | | 75-100% | 25-75% | 10-25% |
| Alkalinity (carbonate) | C(+4) | HCO3- | — | — |
| Aluminum | Al(+3) | Al(OH)4- | — | — |
| Antimony | Sb(+3) | — | Sb(OH)3, HSbO2, Sb2S4-2 | — |
| Arsenic | As(+3) | H3AsO3 | — | — |
| Barium | Ba(+2) | Ba+2 | — | — |
| Beryllium | Be(+2) | — | BeOH+, Be(OH)2 | — |
| Boron | B(+3) | H3BO3 | — | — |
| Bromide | Br(-1) | Br- | — | — |
| Cadmium * | Cd(+2) | Cd(HS)2 | — | — |
| Calcium | Ca(+2) | Ca+2 | — | — |
| Chloride | Cl(-1) | Cl- | — | — |
| Chromium * | Cr(+3) | Cr(OH)2+ | — | Cr(OH)3 |
| Cobalt * | Co(+2) | Co+2 | — | — |
| Copper * | Cu(+1) | Cu(S4)2-3 | — | CuS4S5-3 |
| Fluoride | F(-1) | F- | — | — |
| Iron * | Fe(+2) | Fe+2 | — | — |
| Lead * | Pb(+2) | Pb(HS)2 | — | — |
| Lithium | Li(+1) | Li+ | — | — |
| Magnesium | Mg(+2) | Mg+2 | — | — |
| Manganese | Mn(+2) | Mn+2 | — | — |
| Mercury * | Hg(0) | Hg | — | — |
| Molybdenum * | Mo(+6) | MoO4-2 | — | — |
| Nickel * | Ni(+2) | Ni+2 | — | NiHCO3+, NiCO3 |
| Nitrogen | N(-3) | NH4+ | — | — |
| Phosphorus * | P(+5) | HPO4-2 | — | H2PO4- |
| Potassium | K(+1) | K+ | — | — |
| Selenium * | Se(-2) | HSe- | — | Ag2Se |
| Silica | Si(+4) | H4SiO4 | — | — |
| Silver * | Ag(+1) | Ag2Se | — | — |
| Sodium | Na(+1) | Na+ | — | — |
| Strontium | Sr(+2) | Sr+2 | — | — |
| Sulfate * | S(-2) | HS- | — | — |
| Thallium | Tl(+1) | Tl+ | — | — |
| Tin | Sn(+4) | Sn(OH)6-2 | — | — |
| Uranium * | U(+4) | U(OH)4 ** | — | — |
| Vanadium * | V(+3) | V(OH)3 | — | — |
| Zinc * | Zn(+2) | ZnS(HS)- | — | — |
| Radioactive elements (speciation calculated using PHREEQCdata025.dat) | | | | |

| Analyte (sorted alphabetically by name) | Dominant oxidation state | Dominant species (Percent of total) | | |
|---|---|---|---|---|
| | | 75-100% | 25-75% | 10-25% |
| Americium * | Am(+3) | — | AmCO3+ | Am(OH)2+, AmOH+2 |
| Cerium | Ce(+3) | CeCO3+ | — | Ce(CO3)2- |
| Cesium | Cs(+1) | Cs+ | — | — |
| Neptunium * | Np(+4) | Np(OH)4 | — | — |
| Plutonium * | Pu(+3) | PuOH2+2 | — | Pu+3 |
| Radium | Ra(+2) | Ra+2 | — | — |
| Technetium * | Tc(+4) | TcO(OH)2 | — | — |

Data base: Minteq.v4.dat (except as noted)

* Aqueous species of this element are expected to be well below detection limits under the modeled condition, due to its likely precipitation as indicated in Table B-7.

** The contribution of U(OH)5- to uranium speciation is assumed to be negligible, as recommended by Langmuir (1997, p. 501).

Table B-6. Geochemical Speciation for Bounding Case 5: Intermediate Perched Zones, Methanogenic Conditions

| Analyte (sorted alphabetically by name) | Dominant oxidation state | Dominant species (Percent of total) | | |
|---|---|---|---|---|
| | | 75-100% | 25-75% | 10-25% |
| Alkalinity (carbonate) | C(+4) | HCO3- | — | — |
| Aluminum | Al(+3) | Al(OH)4- | — | — |
| Antimony | Sb(+3) | Sb2S4-2 | — | — |
| Arsenic | As(+3) | H3AsO3 | — | — |
| Barium | Ba(+2) | Ba+2 | — | — |
| Beryllium | Be(+2) | — | BeOH+, Be(OH)2 | — |
| Boron | B(+3) | H3BO3 | — | — |
| Bromide | Br(-1) | Br- | — | — |
| Cadmium | Cd(+2) | Cd(HS)2 | — | — |
| Calcium | Ca(+2) | Ca+2 | — | — |
| Chloride | Cl(-1) | Cl- | — | — |
| Chromium | Cr(+3) | Cr(OH)2+ | — | — |
| Cobalt | Co(+2) | Co+2 | — | — |
| Copper | Cu(+1) | Cu(S4)2-3 | — | CuS4S5-3 |
| Fluoride | F(-1) | F- | — | — |
| Iron | Fe(+2) | — | Fe+2, Fe(HS)2 | — |
| Lead | Pb(+2) | Pb(HS)2 | — | — |
| Lithium | Li(+1) | Li+ | — | — |
| Magnesium | Mg(+2) | Mg+2 | — | — |
| Manganese | Mn(+2) | Mn+2 | — | — |
| Mercury | Hg(+2) | HgHS2- | — | — |
| Molybdenum | Mo(+6) | MoO4-2 | — | — |
| Nickel | Ni(+2) | Ni+2 | — | — |
| Nitrogen | N(-3) | NH4+ | — | — |
| Phosphorus | P(+5) | — | HPO4-2, H2PO4 | — |
| Potassium | K(+1) | K+ | — | — |
| Selenium | Se(-2) | — | HSe-, Ag2Se | — |
| Silica | Si(+4) | H4SiO4 | — | — |
| Silver | Ag(+1) | Ag2Se | — | — |
| Sodium | Na(+1) | Na+ | — | — |
| Strontium | Sr(+2) | Sr+2 | — | — |
| Sulfate | S(-2) | — | HS-, H2S | — |
| Thallium | Tl(+1) | Tl+ | — | — |
| Tin | Sn(+4) | Sn(OH)6-2 | — | — |
| Uranium | U(+4) | U(OH)4 ** | — | — |
| Vanadium | V(+3) | V(OH)3 | — | — |
| Zinc | Zn(+2) | ZnS(HS)- | — | — |

| Analyte (sorted alphabetically by name) | Dominant oxidation state | Dominant species (Percent of total) | | |
|---|---|---|---|---|
| | | 75-100% | 25-75% | 10-25% |
| Radioactive elements (speciation calculated using PHREEQCdata025.dat) | | | | |
| Americium * | Am(+3) | — | AmCO3+ | AmOH+2, Am(OH)2+ |
| Cerium | Ce(+3) | CeCO3+ | — | — |
| Cesium | Cs(+1) | Cs+ | — | — |
| Neptunium * | Np(+4) | Np(OH)4 | — | — |
| Plutonium * | Pu(+3) | — | PuOH+2, Pu+3 | — |
| Radium | Ra(+2) | Ra+2 | — | — |
| Technetium * | Tc(+4) | TcO(OH)2 | — | — |

Data base: Minteq.v4.dat (except as noted)

* Aqueous species of this element are expected to be well below detection limits under the modeled condition, due to its likely precipitation as indicated in Table B-7.

** The contribution of U(OH)5- to uranium speciation is assumed to be negligible, as recommended by Langmuir (1997, p. 501).

Table B-7. Trace metals and Radioactive Elements Expected to be Below Method Detection Limits under Iron-Reducing or Methanogenic Conditions due to Precipitation of Mineral Phases

| Analtye[a] | Mineral dissolution may be more significant than precipitation[b] | Metal hydroxide or oxide | Fe(II) or Cr(III) mixed metal oxide | Sulfide | Selenide | Phosphate | Other (e.g., silicate) |
|---|---|---|---|---|---|---|---|
| Antimony | X | | | | X | | |
| Arsenic | X | | | X | | | X |
| Barium | | | | | | | X |
| Beryllium | | | | | | | |
| Boron | | | | | | | |
| Cadmium | | | X | X | X | | |
| Chromium | | X | X | | | | |
| Cobalt | X | | X | X | | | [c] |
| Copper | X | X | X | X | X | | |
| Iron | X | X | X | X | X | | X |
| Lead | X | | | X | X | | |
| Manganese | X | | | | | | |
| Mercury | | | | X | X | | |
| Molybdenum | X | | | X | X | | |
| Nickel | X | | X | X | X | | X |
| Selenium | | | | | X | | |
| Silver | | | | X | X | | |
| Strontium | X | | | | | | X |
| Thallium | | | | | | | |
| Uranium | | X | | | | | X |
| Vanadium | | X | | | | | |
| Zinc | X | | | X | X | | |
| Radioactive elements (mineral saturations calculated using *PHREEQCdata025.dat*) | | | | | | | |
| Americium | | | | | | [c] | |
| Cerium | X | | | | | [c] | |
| Cesium | | | | | | | |
| Neptunium | | X | | | | | |
| Plutonium | | [c] | | | | X | |
| Radium | | | | | | | |
| Technetium | | X | | | | | |

[a] Trace metals included in modeling but not evaluated: Al, Li, Sn

[b] Based upon significant shifts in mineral saturation indices from oversaturation for oxic conditions to undersaturation under reducing conditions, modeling results support the hypothesis that, for some reducing environments, mineral dissolution is likely to be more significant than mineral precipitation in controlling elemental concentrations and speciation for these trace metals in local groundwaters. However, it may be difficult to separate contributions from dissolution versus those from desorption when evaluating analytical data for these effects.

[c] This mineral phase is supersaturated to the same degree for the base case (oxic conditions). Hence, the solubility of this mineral phase is not directly affected by redox conditions.