INL/EXT-10-19385
Revision 1

# Assessment of Geochemical Environment for the Proposed INL Remote-Handled Low-Level Waste Disposal Facility

November 2011


The INL is a U.S. Department of Energy National Laboratory
operated by Battelle Energy Alliance

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# Assessment of Geochemical Environment for the Proposed INL Remote-Handled Low-Level Waste Disposal Facility

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Prepared for the
U.S. Department of Energy
Office of Nuclear Energy
Under DOE Idaho Operations Office
Contract DE-AC07-05ID14517

# ABSTRACT

Conservative sorption parameters have been estimated for the proposed Idaho National Laboratory Remote-Handled Low-Level Waste Disposal Facility. This analysis considers the influence of soils, concrete, and steel components on water chemistry and the influence of water chemistry on the relative partitioning of radionuclides over the life of the facility. A set of estimated conservative distribution coefficients for the primary media encountered by transported radionuclides has been recommended. These media include the vault system, concrete-sand-gravel mix, alluvium, and sedimentary interbeds.

This analysis was prepared to support the performance assessment required by U.S. Department of Energy Order 435.1, "Radioactive Waste Management." The estimated distribution coefficients are provided to support release and transport calculations of radionuclides from the waste form through the vadose zone. A range of sorption parameters are provided for each key transport media, with recommended values being conservative. The range of uncertainty has been bounded through an assessment of most-likely-minimum and most-likely-maximum distribution coefficient values. The range allows for adequate assessment of mean facility performance while providing the basis for uncertainty analysis.

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# ACRONYMS

| | |
|---|---|
| ATR | Advanced Test Reactor |
| CDP | cellulose degradation products |
| CEC | cation exchange capacity |
| CSH | calcium-silica-hydroxide |
| DOE | Department of Energy |
| INL | Idaho National Laboratory |
| $K_d$ | distribution coefficient (also known as sorption or partition coefficient) |
| LLW | low-level waste |
| NRF | Naval Reactors Facility |
| RH | remote-handled |
| RWMC | Radioactive Waste Management Complex |

# Assessment of Geochemical Environment for the Proposed INL Remote-Handled Low-Level Waste Disposal Facility

## 1. BACKGROUND

Since 1952, all remote-handled low-level waste (RH-LLW) generated at the Idaho National Laboratory (INL) has been disposed of at the Subsurface Disposal Area of the Radioactive Waste Management Complex (RWMC). In anticipation of closure of RWMC, INL is proposing to establish a new RH-LLW disposal facility for the disposal of resins, activated metals, and a small fraction of miscellaneous surface contaminated debris. An important part of the decision process requires an evaluation of groundwater impacts determined largely by the release rate of radionuclides from the initial waste form and their subsequent transport through the vault system, vadose zone, and into the aquifer. Transport of radionuclides is determined by advection, dispersion, and sorption onto solid surfaces. The focus of this report is the determination of the geochemistry along the transport pathway that controls sorption parameters and the estimation of sorption parameters.

### 1.1 Objective

The objective of this document is to provide estimated distribution coefficients ($K_d$) for use in transport models of the RH-LLW disposal facility. These $K_d$s reflect the boundaries of system performance; therefore, a range of potential values is provided. The RH-LLW facility is not a simple system. As shown in Figure 1, the system consists of a sequence of zones where aqueous constituents transit through different infiltration zones while interacting with different gaseous components, solid matrices, and energy fluxes. The chemical and physical behavior of each of these zones and components will vary over time. To reach the waste (orange dot), water has to pass through an engineered cover, a cement vault, and a steel waste container. To reach the aquifer, *contaminated* water has to exit the container and vault, pass through underlying sediment (alluvium), and pass through multiple layers of fractured basalt and sedimentary interbeds. Each of these "layers" has unique geochemical and hydrologic properties and will impact the solution and any entrained waste in separate ways.

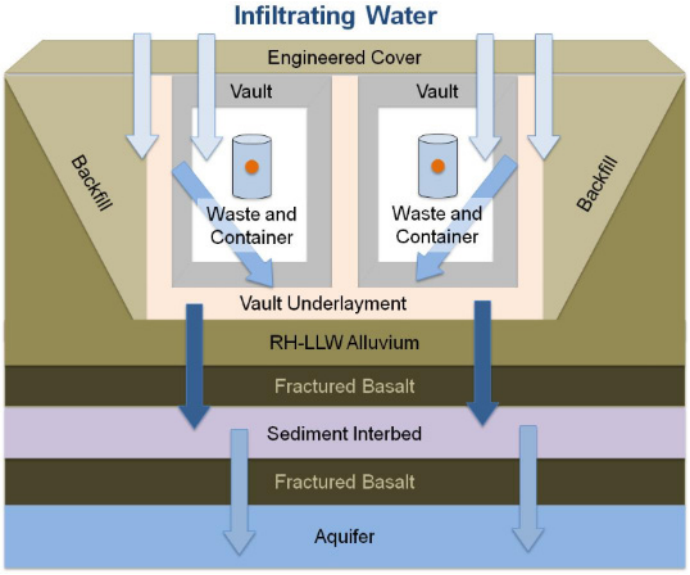


Figure 1. Diagram of the contaminant-waste-repository system at the remote-handled low-level waste facility. Arrows indicate solution transport and zones of alteration of solution properties.

Bounding the potential $K_d$s requires that these separate impacts be evaluated. This report will provide six pieces of information that are needed to support the performance assessment for the RH-LLW facility:

1. *Estimated $K_d$s and bounds of uncertainty for release of radionuclides from anion-exchange resins.* The release of radionuclides from ion-exchange resins will be assumed to occur via linear equilibrium adsorption and will be modeled using an equilibrium $K_d$. The cement vaults will degrade over time, and the pore-water chemistry will evolve over time in response to concrete degradation. Geochemical conditions will range from background conditions to high-pH, high-ionic strength conditions and then revert to near background conditions over time. Also, the resins will slowly degrade via oxidative radiolytic processes, losing their functionality and anion exchange capacity and releasing predominantly gaseous reaction products that may impact steel liner corrosion. As resin properties and pore-water chemistry changes, the release $K_d$s for anions on ion-exchange resins will change. This report provides (1) an assessment of the range of pore-water chemistries and resin properties that are anticipated to occur, and (2) estimated $K_d$ ranges that correlate with those properties.
2. *Assessment of metal corrosion in the vault environment and the impact of metal corrosion on the release $K_d$ of co-located resins*. Waste in the RH-LLW disposal facility is initially contained in carbon steel and stainless steel liners placed within the reinforced concrete vaults. Metal waste is primarily associated with activated metals (stainless steel, zircaloy, or inconel). The potential impact of high pH and resin radiolysis on corrosion of metal reactor parts, rebar, and enclosing steel liners; and the combined effect of high pH, resin radiolysis, and metal corrosion on the $K_d$ of resins are evaluated.
3. *Estimated $K_d$ values that can describe radionuclide sorption to cement surfaces in the vault system.* Contaminated solution that escapes from the waste containers will interact with cement surfaces at the bottom of the vault. Estimated $K_d$ values for radionuclide interaction with cement surfaces are provided.
4. *Estimated $K_d$ values and bounds of uncertainty that can describe radionuclide sorption to underlying sand and alluvial materials under "native" conditions*. Radionuclides will adsorb to sand and native alluvium materials beneath the vault. Information is provided to assess how radionuclides would adsorb to these materials if the overlying cement vault did not impact solution composition in the sediment.
5. *Estimated $K_d$ values and bounds of uncertainty that can describe radionuclide sorption in underlying sand and alluvial materials under native conditions when solution chemistry has been altered by the presence of a large mass of overlying cement and when an infiltrating solution(s) contains cellulose degradation products*. Groundwater interaction with the cement vault at the RH-LLW facility will likely raise pH and solution ionic strength above what they would be if the vault were not present. This will have a corresponding impact on the sorption $K_d$ for these materials. The potential impact of cement leachate on the $K_d$ for radionuclide interaction with native alluvium materials is evaluated.
6. *Estimated $K_d$ values and bounds of uncertainty that can describe radionuclide sorption in interbeds below the first basalt layer*. Radionuclides will adsorb to interbed sediment. Information is provided to assess how radionuclides would be expected to adsorb to these materials.

## 1.2 Conceptual Approach

The modeling approach used to evaluate exposure risk at the RH-LLW facility uses a constant $K_d$ to describe contaminant sorption to materials in and beneath the vault environment. The $K_d$ is an approximate measure of sorption and is defined as the ratio of the quantity of the adsorbate (i.e., radionuclides, cations, and anions) adsorbed per unit mass of solid to the quantity of the adsorbate remaining in solution at equilibrium:

$K_d$ (mL/g) = adsorbed concentration (g/g)/aqueous concentration (g/mL). (1)

It is important to note that a $K_d$ is only applicable to the specific combination of adsorbent and aqueous chemical conditions (e.g., adsorbate concentration, solution/electrolyte matrix, and temperature) for which it has been determined. Consequently, $K_d$ is not a physical constant that is rigorously founded in geochemical principles. It is a generalization of bulk system properties that can provide useful estimates of minimum sorption under a specific set of circumstances if environmental conditions are closely matched.

Describing the $K_d$ of a specific species in terms of this simple ratio assumes that all adsorption sites and reaction processes are the same and have the same reactivity toward a given radionuclide; reactivity does not change with solution chemistry; the system is in thermodynamic equilibrium; the reaction is fully reversible; and activity of the adsorption sites and aqueous ions is the same as in the experimental system under which they were determined. While none of these assumptions is strictly correct, a $K_d$ can be used to give a rough estimate of the minimum anticipated contaminant retention if solution conditions are relatively constant and adsorption/nucleation sites are in great excess with respect to the concentration in the water phase. This approach is typically considered to be conservative in groundwater transport analyses because it predicts more transport than would most likely occur. It can be used to define the limiting conditions for the RH-LLW disposal facility because of very low (slow) infiltration through the facility leading to very slowly changing conditions. Even so, single $K_d$ value cannot describe contaminant sorption for a given radionuclide under all physicochemical conditions within a given substrate, and different values should be used to describe specific sets of geochemical conditions.

Slow changing conditions and lack of facility-specific data precludes the use of an integrated geochemical model that accounts for all transitions and hydrogeochemical processes that would allow back-calculating partition coefficients (i.e., $K_d$). Further, the overall geometric complexity precludes the application of multidimensional models. Therefore, the flow system is conceptualized as a series of one-dimensional layers with each layer considered separately. In this implementation, the output from overlying layers provides the input to underlying layers. There also is insufficient data to evaluate each layer in the same way. Insufficient site-specific data prevents the use of first principle calculations to describe each component of the system. Thus, a blend of first principle calculations and empirical data are used to define solution composition in each layer of the system. $K_d$ values are then estimated on the basis of solution composition.

- *For release of anions from resins* – $K_d$ values are estimated from anion charge concentration in solution and the exchange capacity of the resins. Anion charge concentration is estimated based on a range of scenarios regarding native alluvium water concentration, infiltration rate, cement degradation, and steel corrosion. A range of values is given for different sets of assumptions.
- *For sorption to cement surfaces* – $K_d$ values are adopted from the literature.
- *For sorption to sediment surfaces* – $K_d$ values are estimated by applying an empirical cement leachate impact factor to $K_d$ values for sediment under "native" conditions. Cement leachate calculations are used to determine which combinations of cement leachate and groundwater mixing scenarios could create "cement-impacted" groundwater conditions beneath the RH-LLW vault. $K_d$ values for "native" conditions are from direct measurements where possible and adopted from the literature for cases where direct measurements are not available. To account for the potential impact of organic degradation in overlying waters, empirical factors for the impact of cellulose degradation products (CDP) on $K_d$ values also are provided. These CDP factors are derived from the scientific literature.

The impact of cement leaching on solution composition is modeled from thermodynamic principles using batch-mode reactive transport assumptions and generalized chemical properties of Portland cement. Batch mode calculations are used to provide estimates of the bounding conditions. Steel corrosion rates are adopted from empirical data gathered under native soil conditions at INL (e.g., near-neutral pH). The impact of cement and CDP on radionuclide sorption to the underlying alluvium sediment is estimated from a combination of empirical studies and literature reports. These impacts cannot be modeled from

first principles with currently available data. Measurements of the concentration of surface adsorption sites for INL alluvium sediment are not available, and the response of the sorptive properties to the anticipated shifts in solution pH and ionic strength has not been measured. However, direct measurements of cation exchange capacity (CEC) for alluvium sediment underlying the RH-LLW disposal facility are available. Generalized contaminant sorption processes can be inferred from groundwater chemistry, knowledge of contaminant chemistry, and mineralogical data collected from other locations at the site that have similar bulk sediment properties (e.g., CEC and grain size).

Inside the vault, cement leaching and degradation will alter solution chemistry. This has two major effects. First, cement leaching increases solution pH. This slows the rate of corrosion of steel waste containers (liners) and alters the aqueous solubility of radionuclides. Second, cement leaching increases the ionic strength of the infiltrating solution. If this increase in anion-charge concentration persists as solution infiltrates into the steel liners, then a higher anion charge concentration will reduce the $K_d$ that can be used to define the release of anion radionuclides from waste anion-exchange resins. *To assess this potential impact, a batch-mode geochemical model is used to estimate the anion-charge concentration of a solution that reacts with cement surfaces prior to infiltrating into corroding steel waste containers*.

In the sediment beneath the vault, cement leaching has a number of counterbalancing effects on radionuclide transport. Elevated pH will tend to decrease the solubility of metallic radionuclides and increase the extent of sorption (e.g., higher $K_d$). However, pH also impacts carbonate speciation and colloid formation, potentially lowering $K_d$ values for metals whose speciation is impacted by these processes. Nuclides of primary interest to the RH-LLW disposal facility are C-14, I-129, Tc-99, and U-238, and are generally not impacted by colloid formation. For poorly sorbing anions (e.g., Cl, I, and Tc), cement degradation can increase solution ionic strength and decrease sorption, leading to a lower $K_d$. The magnitude of these impacts can vary significantly over the range of pH and ionic strength that cement leaching can create. Describing these changes from first principles, for a wide range of radionuclides, is a complex task with many interdependencies. *Here, there is insufficient data to model these processes from first principles, but a geochemical model is provided to help define the system so that appropriate empirical estimates can be adopted from the literature*.

### 1.2.1 Geochemical Model of Cement Leaching

Solution chemistry has been estimated using a simplified geochemical model to estimate the potential impact of cement leaching and metal. The geochemical model for cement used batch-mode calculations that try to capture the key properties of cement-water systems as cement dynamically ages (Figure 2).

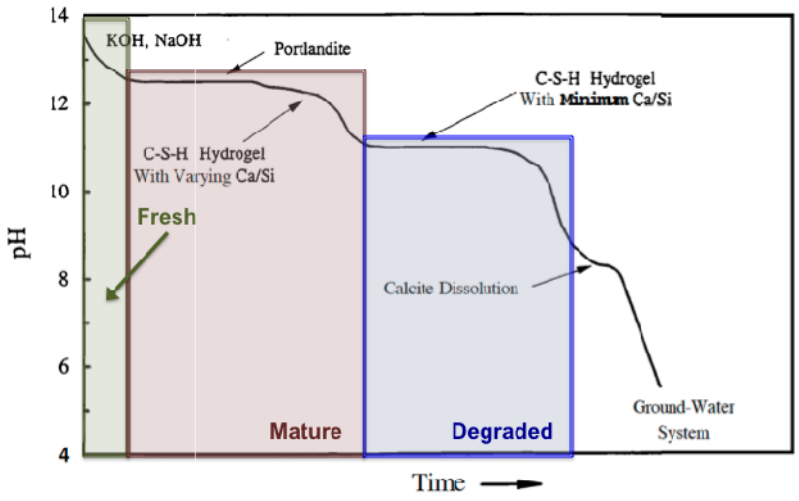


Figure 2. Time-dependent pH changes in a cement-water system after water is added to dry cement. Plot is adapted from Krupka and Serne (1998) to show regions of fresh, mature, and degraded cement.

In the first stage of cement dissolution, soluble hydroxide salts leach out of "fresh" cement, maintaining pH above 13 and greatly increasing solution ionic strength. In the second stage, water dissolves portlandite in "mature" cement, with ionic strength being reduced and pH ranging from 11 to 13. In the final stage, termed "degraded" cement, all portlandite has been replaced with calcium carbonate minerals and water slowly dissolves the calcium-silica-hydroxide (CSH) gel. Ionic strength is only slightly higher than natural levels and pH typically ranges from 9 to 11. The time axis shown in Figure 2 can be correlated to the number of water exchange cycles, or pore-volumes (PV) of fluid passing through the cement. The time (t) necessary to exchange fluid from one concrete pore volume (PV) is related to the total influx ($Q_{total}$ $cm^3$/sec) and the porosity ($\phi$) by: $t=PV*\phi/Q_{total}$. Based on data provided by Berner (Table 7, 1992), the relationship between pH, PV, and dissolution stage for a specific cement and infiltration rate is as follows:

- *Fresh cement.* 1 – 523 pore volumes, pH > 12.0
- *Mature cement.* 523 – 1,097 pore volumes, pH 11.2 – 12.0
- Mature cement transitioning to degraded cement. 1,097 – 4,413 pore volumes, pH 10.3 – 11.2
- *Degraded cement.* 4,413 – 6,650 pore volumes, pH 7.4 – 10.3.

In general, it is difficult to chemically define the pH ranges corresponding to the dissolution stages for generic cement and particularly for degraded cement. Most available literature describes reactions between water and fresh cement or water and mature cement. Furthermore, most literature studies that describe solution composition utilize batch-mode calculations, where the entire mass of cement is available for reaction with solutions. Consequently, there are few sources of confirmatory analyses to bound model calculations that describe the impact of cement leaching on solution chemistry under a reactive transport scenario.

Determining the time corresponding to each dissolution stage for the RH-LLW disposal facility would require employing a transport model, where fluid advectively flows across a slowly degrading cement surface and solution inside internal cement pores interacts with the advecting "external" solution via diffusive processes. This approach could capture the dynamics of the system and yield reasonably accurate predictions. However, this would require the specific cement composition, a detailed geometric model including the initial porosity, developing secondary porosity and cracks, porosity between the cement vaults and steel waste liners, and waste components contained within the steel waste liners. In this model, infiltrating water would pass through the bulk cement pore space and along the interfaces of the secondary porosity and cracks. This flow system would be more complex than the experiments of Berner (1992), making a direct comparison between pore volume and time problematic. Given the lack of specific cement composition, geometric complexity, and the correspondingly higher number of parameters that must be assumed in order to conduct these calculations, all geochemical calculations involving cement are conducted in batch mode. This use of batch mode calculations broadens the range of potential solution compositions beyond what would be expected under more realistic assumptions, and generates a comparably wider range of potential $K_d$ values. However, by providing a greater range that extends to improbably low or improbably high $K_d$ values, there is correspondingly greater certainty that the system will perform within the boundaries established. The objective of this study is to provide a range of $K_d$ values that maximizes the certainty that the RH-LLW facility will perform safely within established boundary conditions, not to estimate the most likely outcome of hydrogeochemical processes. Consequently, the use of batch mode calculations to provide bounding estimates of $K_d$ values fulfills the objective of this work

Applying batch mode calculations for steel corrosion and cement degradation requires knowledge of corrosion rates and average residence time of infiltrating water within the cement vault and waste zone. These, in turn, depend on assumptions regarding the average infiltration rate and the corrosion rate of metal reactor parts and waste containers. The infiltration rate is anticipated to vary over time, and

sensitivity calculations for the performance assessment will need to consider a range of potential corrosion rates. Each of these scenarios requires applicable $K_d$ values for release of radionuclides from the resins, and for sorption to surfaces in the underlying strata. Estimates of infiltration rates, corrosion rates, and cement degradation are particularly important for estimating the release $K_d$ from resins This study will provide a table of resin $K_d$ values for infiltration rates of 0.1 cm/year, 0.5 cm/year, 1 cm/year, and 10 cm/year, with applicable estimates for net area of infiltration. For each of the infiltration rates, estimates will be provided for the "minimum" and "maximum" anticipated corrosion rate.

# 2. DETERMINATION OF SOLUTION AND MATERIAL COMPOSITION FOR EVALUATING SORPTION WITHIN THE CEMENT VAULT AND UNDERLYING SEDIMENT

To assess geochemical parameters within the cement vault and underlying alluvium, scenarios have been developed to bound conditions under which water could infiltrate into the vault and steel liners (e.g., waste containers) and then out of the vault and into the underlying alluvium. They include scenarios that are improbable and those that are more likely to occur. For each of the scenarios, the water composition that infiltrates through cement and corroding steel is modeled using thermodynamic calculations based on assumptions about the water and solid phase composition of the relevant system layers. Model calculations are only used to estimate the impact of cement leaching and steel corrosion on solution composition. $K_d$ values for release of anion radionuclides from anion-exchange resins and interaction with alluvium sediment are then estimated analytically on the basis of solution composition and the materials' physical properties. This section describes how the solution and solid-phase composition is defined for each layer of the system.

## 2.1 Conceptual Model for Geochemical Evolution at the Remote-Handled Low-Level Waste Facility

During the first 50 years, radioactive waste will be deposited in steel liners emplaced into concrete vaults at the RH-LLW facility. The facility will be actively maintained. Snow will be removed and rainwater managed to reduce water contact with the waste containers. Water that does enter the facility will come in contact with the cement walls of the repository, initiating cement degradation. During this period, the total infiltration from precipitation will likely average 18 cm/yr through the facility top at land surface. The sand infill is estimated to cover ~10% of the areal footprint and have ~20% porosity, reducing the net porous media porosity to ~2%. The sand infill will be much more permeable than the concrete vault plugs, and most of this precipitation would be expected to migrate through the sand infill rather than through the concrete unless cracks formed in the vault plugs. At a net porosity of 2% and precipitation of 18 cm/yr during the first 50 years, the total infiltration equates to 45 sand-infill PVs. At 31% total concrete porosity (primary porosity plus secondary porosity representing the potential development of micro fissures), total infiltration equates to 6.5 concrete PVs, assuming all infiltrating water passes through the concrete, which is highly unlikely given the permeability contrast between sand and concrete.

Prior to reaching the bottom of the vault system, liquid water infiltrating into the vault would have to pass either through the concrete porosity, along the external surfaces between the sand infill and concrete vaults, or through the sand infill. Given a maximum exposure of 6.5 pore volumes, it is unlikely that exposed concrete surfaces would degrade to a mature state during this initial 50-year period. The majority of the cement should still be in the fresh stage. Surface wash from the cement will likely alter solution chemistry in the underlying alluvium (discussed in subsequent sections), but is unlikely to significantly impact the internal structure of the cement. It should also be noted that the bottom of the vault will contain drain holes that would enable moist soil-gas to migrate upward into vaults. This would enable water to condense on cooler surfaces, accumulate, and eventually drain out of the bottom.

During this initial period, three different waste forms will be emplaced in different configurations. These waste forms are activated metals, anion-exchange resins, and miscellaneous debris. In most cases, anion exchange resins will be stored in vaults that contain two resin containers. However, some resins may be co-located with activated metals containers and receive a higher radiolytic dose. Radiolysis will degrade the resin beads, with greater dose equating to greater loss of chemical functionality, faster release of degradation products, faster corrosion, and lower release $K_D$. This report will consider both cases.

After 50 years, an engineered cover will be placed over the RH-LLW repository. The engineered cover is anticipated to reduce total infiltration to 0.1 cm/year during the first 500 years, increasing to 1 cm/yr at and beyond 1,000 years. During the first 1,000 years, less than 80 total pore volumes will likely enter the vault-sand system, with approximately 88% of this volume passing through the sand infill and ~12% moving through cement. Liquid water infiltrating into the vault system will need to pass through the engineered cover and the concrete vault. Condensate generated in the vault would likely form on the concrete. Liquid water would have to penetrate the waste container before reaching the waste. To reach the aquifer, contaminated water would have to leave the waste container, pass through the floor of the vault or drain holes, traverse the vault base layer and alluvium, and then pass through multiple layers of basalt and sedimentary interbeds. Vapor-phase water could not transport any radionuclides that do not exist in a vapor phase (i.e., tritium). For the purposes of this assessment, all water entering the waste containers is assumed to be liquid water. For liquid water, each media encountered will alter the chemical composition of the infiltrating water. A summary of these influences is provided in Table 1.

Table 1. Factors influencing geochemical composition of reactive zones within the cement vault.

| Reactive Zone | Geochemical Influences | Considerations for $K_d$ Calculations |
|---|---|---|
| Engineered Cover | Infiltrating rainwater and snowmelt, solubility of chloride, and sulfate salts contained in the cover material | Initial solution condition assumes measured range of INL shallow groundwater compositions |
| Vault Interior | Native alluvium water, cement, carbon steel, and stainless steel | Water composition, cement reactions, steel corrosion, and residence time of water |
| Waste Zone | Vault interior water, physiochemical properties of resins, radiolytic decay of anion resins, corrosion of carbon steel, stainless steel and steel alloys, and waste source term | Water composition, steel corrosion, radiolytic loss of anion exchange capacity, physical properties of source term, and residence time of water within the waste zone |
| Vault Underlayment | Vault interior water, waste source term, native alluvium water, and sand/gravel | Water composition, cement reactions, and physiochemical properties of sand/gravel |
| Alluvium | Vault interior water, waste source term, native alluvium water, and native alluvium material | Water composition, mixing from vault underlayment and alluvium material, and physical properties of alluvium material |
| Sedimentary Interbeds | RH-LLW alluvium water, sediment interbed water, and sediment interbed | Water composition and physical properties of interbed sediment |
| Basalt | RH-LLW alluvium water and sediment interbed water | Assumed to be non-reactive |

An alternate way to visualize this system is provided in Figure 3. The following sequence of geochemical reactions that establish the composition of solution that comes in contact with the waste encased within steel liners and then exits the vault correspond with the numbered arrows in Figure 3:

1. Engineered cover comprised of alluvial materials controls the composition of the water that comes into contact with the top of the cement vault.
2. Infiltrating water reacts with the mineral components of cement as the water infiltrates through cement pores and cracks in the vault or water vapor condenses on cement surfaces.
3. Water leaving the cement contacts the steel liners. Steel corrosion further alters solution chemistry.

4. Water that has reacted with cement and corroding steel reacts with the waste source (this water determines the release Kd).
5. Radionuclide contaminants in water that escape from the liners adsorb to cement surfaces at the bottom of the vault.
6. After water exits the bottom of the vault, it comes in contact with the underlayment material (sand and gravel); chemical retention within this zone will depend on the extent of lateral mixing and the degradation of the outer cement surfaces of the vault.
7. After water exits the underlayment material, it will come in contact with native alluvium. Chemical retention within this zone will depend on the same factors as within the vault underlayment. However, the soils will have different geochemical and hydrological properties than water in the vault underlayment and surrounding native alluvium.

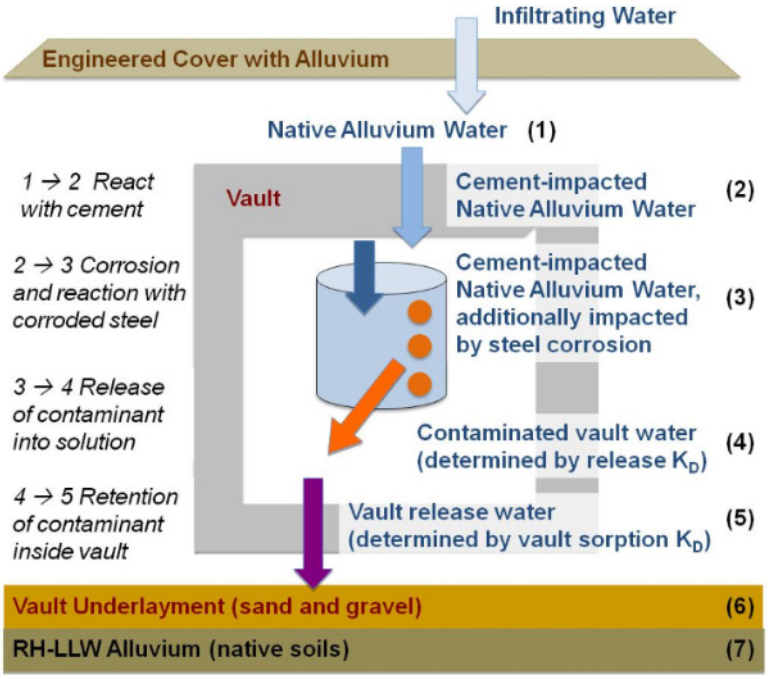


Figure 3. Detail of geochemical reaction sequences in the remote-handled low-level waste disposal facility above the first basalt contact. Each numbered arrow in Figure 3 corresponds to a type of water that is created during the process of infiltration and its reaction with various vault constituents.

After water exits the remaining alluvium materials, it passes through a sequence of basalt and sedimentary interbeds that are discussed separately in subsequent sections. Each of the water types in Figure 3, and the corresponding geochemical conditions that determine their composition, are discussed in this section (in sequential order).

## 2.2 Chemistry of Infiltrating Alluvium Water (Figure 3, Point #1)

The first factor that impacts the composition of water infiltrating into steel liners in the vault is the composition of native alluvium water that forms as rain and snowmelt infiltrate through alluvial soils. Infiltrating liquid water (e.g., that which is not transported via the vapor phase) will have to equilibrate with either the engineered cover or backfill materials prior to encountering the vault (Figure 1). Backfill materials have not yet been finalized, but will likely consist of alluvial sediment from the RH-LLW site that was excavated prior to installation of the cement vaults. Similarly, it is likely that the majority of material used in the engineered cover will be comprised of alluvial materials.

The water composition that results as precipitation infiltrates into surficial sediment will likely be emulative of interstitial water existing in areas of the INL site that have not been impacted by historic site operations. Measurements of the composition of interstitial water in clean alluvium at INL are scarce, because most monitoring operations focus on contaminated zones, aquifer water, and interbed water. However, a few datasets do exist. The most comprehensive and internally consistent dataset comes from Hull and Bishop (2003, 2004), who evaluated the chemistry of shallow interstitial waters at RWMC to determine the fate of $MgCl_2$ brines that had been applied as dust control agents. Results from their study, for samples not impacted by brines, are summarized in Table 2. These data can be considered to be reasonably emulative of infiltrating INL alluvium water.

Table 2. Composition of `Idaho National Laboratory alluvium water, with variance statistics. Data gathered from shallow lysimeters at the Radioactive Waste Management Complex that have not been impacted by MgCl2 brines (n = 16). Water corresponds to Point #1 in Figure 3.

| Parameter | pH | Ca-aq (mM) | Mg-aq (mM) | Na-aq (mM) | K-aq (mM) | ΣCO2-aq (mM) | Cl-aq (mM) | $SO_4$-aq (mM) | $NO_3$-aq (mM) | cations (meq/L) | anions (meq/L) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Minimum | 6.9 | 0.6 | 0.3 | 1.3 | 0.0 | 1.4 | 0.0 | 0.3 | 0.0 | 9.2 | 9.6 |
| Maximum | 8.0 | 3.1 | 5.0 | 18.0 | 1.9 | 21.8 | 7.5 | 7.3 | 7.9 | 27.7 | 27.3 |
| Median | 7.3 | 1.9 | 2.4 | 7.3 | 0.1 | 7.5 | 1.0 | 1.7 | 0.0 | 13.8 | 13.7 |
| % deviation from median | 5% | 42% | 57% | 84% | 459% | 75% | 237% | 105% | 261% | 51% | 52% |
| Skewness | 0.5 | -0.2 | 0.6 | 0.3 | 3.8 | 1.2 | 1.5 | 1.4 | 2.8 | 0.3 | 0.3 |
| Kurtosis | -0.7 | -1.3 | -0.02 | -1.5 | 14.4 | 1.2 | 1.1 | 2.5 | 7.6 | -1.8 | -2.0 |

The data in Table 2 includes the overall maximum and minimum values and computed median. High percent deviation from the median indicates the presence of at least one outlier. Overall, data in Table 2 indicate that the ion composition of groundwater in surficial sediment is variable, with skewed, non-normal distributions that can be strongly impacted by outliers. Sodium and bicarbonate are the dominant ions. In contrast to individual ions, the sum of all ions (e.g., cations and anions) has a flatter distribution that is notably less skewed. This discrepancy between individual ion distributions and total ion distribution could result from a set of processes that normalize ion content to the dominant ions. Surficial groundwater at INL is variably saturated with respect to calcite, with the median saturation index ranging from 2 to 4, depending on the pH dataset used to calculate aqueous carbonate speciation. Supersaturation with respect to calcite suggests that carbonate mineral precipitation could homogenize groundwater composition prior to encountering the vault. Together, these data provide three possible pore water compositions: minimum, median, and maximum salt composition. The minimum and maximum compositions are used to bracket the composition of liquid water infiltrating into the cement ceiling of the vault.

## 2.3 Infiltration Rate and Residence Time of Water

The geometry of the waste zone and the area of water infiltration is shown in Figure 4. The baseline scenario for the rate of infiltration into the RH-LLW facility (DOE-ID-11421) assumes an infiltration scenario that is as follows:

- *Operations.* Water infiltrates at 18 cm/year during operations, but does not enter the waste zone.
- *Fully functional soil cover*. The soil cover will decrease infiltration to approximately 0.1 cm/year for a period of 500 years.
- *Degrading soil cover*. After 500 years, the soil cover will begin to degrade. Infiltration will increase linearly over 500 years, reaching natural background rates of approximately 1.0 cm/year by 1,000 years after the cover was installed.
- *Natural infiltration*. After 1,000 years, water will infiltrate at background rates (1.0 cm/year).

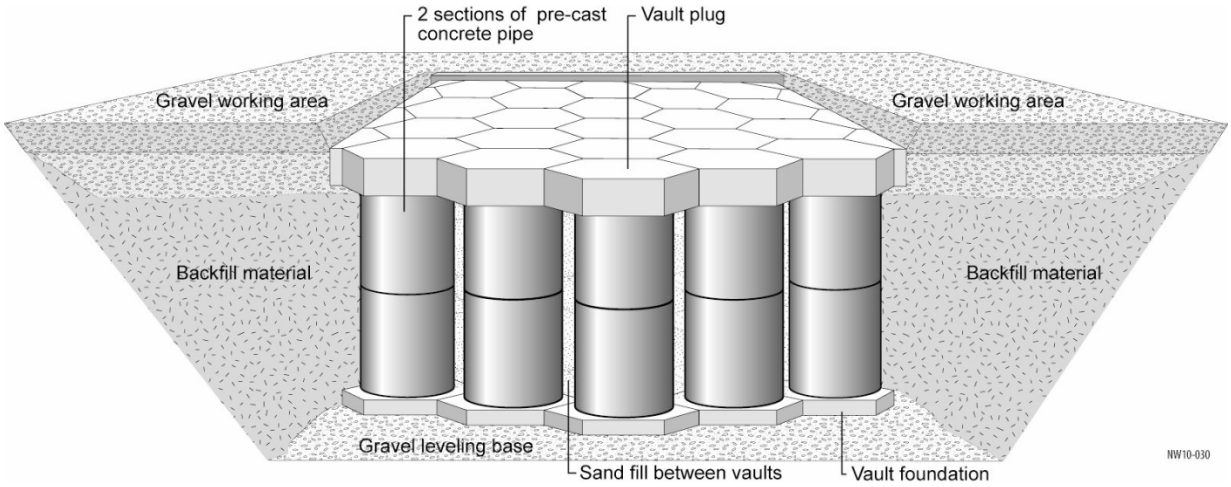


Figure 4. Conceptual drawing of the concrete vault layout. It is assumed that small gaps will exist between the vault plugs.

These time periods dictate the rate at which water will move through the overlying alluvium to reach the top of the vault. Once water encounters the vault, the cement vaults and plugs will alter fluid flow. The cement plugs will initially be impermeable to water and water will be diverted to the sides or focused through the sand infill that separates the concrete vaults and vault plugs. Additionally, some soil moisture will imbibe through the vault walls or through the vault bottoms, condense, and exit the vault as liquid water. As the cement begins to degrade, infiltration through the cement will increase. Over time, the cement will fully degrade, sediment will infill into cracks that form, and water will transit through an ever larger area. These processes will combine to alter the residence time of water within the waste zone and the extent to which the combined action of cement leaching and steel corrosion impact the water chemistry. These changes, in turn, will impact the $K_d$ of radionuclide release from resins.

Water residence time is an independent variable in the $K_d$ calculations and can be estimated from assumptions concerning the net infiltration rate, the percentage of the total waste zone area that is permeable to water, sediment hydraulic properties, and the time period for over which the assumptions apply. Residence time (years) is calculated from the ratio of the total linear distance traveled by water (cm) to the effective infiltration rate (cm/year). Total linear distance is the product of the depth of the waste zone and the assumed porosity. The effective infiltration rate is the product of the net infiltration rate and the fractional area of infiltration (e.g., proportion of total area through which water infiltrates). If the number of pore volumes is desired instead of water residence time, then this value is calculated from the residence time and the applicable time period. The net infiltration rate, fractional area of infiltration, and applicable time period are assumed for a given scenario. The values assumed for this study and the resultant residence time of water are summarized in Table 3.

Ten scenarios have been developed to bound potential water residence time in the waste zone, using the baseline net infiltration scenarios provided in the performance assessment for the RH-LLW facility (DOE-ID-11421). Scenario 1 assumes that the cap and vault system work as planned and water only infiltrates through 10% of the total area during the 500-year period, including an assumed 5% area for sand infill and 5% through cement (on average, over 500 years). This roughly equates to the proportion of the cement area that contains micro-fissures increasing linearly from 0% at 0 years to 10% after 500 years, for an average of 5%. Scenario 2 continues the assumption that the system works as planned and provides average values for the next 500-year period. The soil cap degrades linearly up until it reaches background infiltration at 1,000 years. The cement vault degrades as it did during the first 500 years, reaching 20% porosity by the 1,000-years timeframe. Scenario 3 is similar to Scenario 2, except that cement begins to degrade faster during the next 500 years reaching 25% porosity by 1,000 years (e.g.,

15% incremental porosity per 500 years). In Scenario 3, the effective area of infiltration is the sum of a 5% sand area and an average 500-year additional porosity of 20%. Scenario 4 is a continuance of Scenario 2 for the next 1,000-year period, with a net infiltration rate of 1.0 cm/year. Cement degrades linearly, gaining an additional 10% porosity every 500 years, reaching 40% porosity after an additional 1,000 years aging (e.g., 2,000 years after soil cap emplacement). Scenario 5 continues Scenario 3 for the next 1,000-year period. Cement degrades similar to Scenario 3, reaching approximately 70% porosity by 2,000 years after soil cap emplacement. Scenarios 6 through 8 assume that the soil cap fails, water ponds, and ponding increases water infiltration to 10 cm/year over the first 500 years. The associated fractional area of infiltration covers a range of cement vault scenarios, ranging from baseline performance to catastrophic cracking and failure. Scenarios 9 and 10 extend Scenarios 6 through 8 for the next 500 years and assume that ponding in the cap fills and returns to background, while cement degradation slows to a rate comparable to Scenarios 2 and 3.

Table 3. Derivation of water residence time from assumptions regarding net infiltration rate, proportion of total waste zone area through which water infiltrates, and applicable time period. All calculations assume 21% porosity of freshly laid concrete, time-dependent secondary porosity to account for the formation of micro-fissures, and 10-m height of waste zone. The assumed fractional area of infiltration (Af) is an estimated average over the applicable time period, assuming 5% sand infill area and linear increases in secondary porosity due to the formation of micro-fissures that may result from cement degradation.

| Scenario Number | Net Infiltration Rate (cm/year) | Total Linear Distance Traveled (cm) | Assumed Fractional area for Infiltration | Effective Infiltration Rate (cm/year) | Estimated Residence Time (years) | Applicable Time Period (years) | Number of Pore Volumes |
|---|---|---|---|---|---|---|---|
| 1 | 0.1 | 260 | 0.1 | 1.0 | 260 | 0 to 500 | 1.9 |
| 2 | 0.5 | 360 | 0.2 | 2.5 | 144 | 500 to 1,000 | 3.5 |
| 3 | 0.5 | 410 | 0.25 | 2 | 205 | 500 to 1,000 | 2.4 |
| 4 | 1 | 510 | 0.35 | 2.8 | 182 | >1,000 | 5.5 |
| 5 | 1 | 660 | 0.5 | 2.0 | 330 | >1,000 | 3.0 |
| 6 | 10 | 260 | 0.1 | 100 | 2.6 | 0 to 500 | 192 |
| 7 | 10 | 410 | 0.25 | 40 | 10.2 | 0 to 500 | 49 |
| 8 | 10 | 510 | 0.35 | 28 | 18 | 0 to 500 | 28 |
| 9 | 5 | 660 | 0.5 | 10 | 66 | 500 to 1,000 | 7.6 |
| 10 | 5 | 810 | 0.65 | 7.7 | 105 | 500 to 1,000 | 4.8 |

* Pore volume ranges for fresh cement, mature cement, mature-degraded transition, and degraded cement are 1 to 523; 523 to 1,097; 1,097 to 4,413; and 4,413 to 6,650, respectively.

As indicated in Column 8, the total number of concrete pore volumes is expected to remain below 200 for all cases considered. If the interpretation provided by Berner (Table 7, 1992) is used, this suggests that fresh cement (1-523 pore volumes) will be encountered throughout the 1,000 year compliance period and well beyond.

Taken together, these assumptions generate a set of infiltration scenarios that vary widely during the initial period of vault aging, but converge as the system obtains an age of about 1,000 years. These scenarios yield five general infiltration cases that help parameterize $K_d$ calculations.

1. First 500 years
    a. *Baseline operations.* Less than 2 pore volumes pass through the vault and each kilogram of water resides in the waste zone for approximately 300 years.
    b. *Catastrophic failure.* Approximately 30 to 190 pore volumes pass through the vault and each kilogram of water resides in the waste zone for 3 to 18 years.

2. Next 500 years (e.g., 500 to 1,000 years after soil cap emplacement)

    c. *Baseline operations.* Approximately 2 to 4 pore volumes pass through the vault and each kilogram of water resides in the waste zone for 150 to 200 years.

    d. *Catastrophic failure.* Approximately 4 to 8 pore volumes pass through the vault and each kilogram of water resides in the waste zone for 60 to 100 years.

3. Beyond 1,000 years (e.g., over 2,000 years after soil cap emplacement)

    e. Approximately 3 to 6 pore volumes pass through the vault every 1,000 years and each kilogram of water resides in the waste zone for 180 to 330 years.

These residence times are used for all corrosion calculations, where the mass of iron that comes into equilibrium with a kilogram of infiltrating water is dependent on the infiltration scenario and the rate of steel corrosion. Calculations that involve chemical thermodynamics assume that each kilogram of water reaches chemical equilibrium with the surrounding system during its period of residence. Reactions involving cement and concrete always assume chemical equilibrium. Corrosion reactions assume that the mass of iron that reacts with water is kinetically determined, but that the entire amount of iron that reacts comes into equilibrium with the infiltrating water.

## 2.4 Evaluation of Chemical Reactions Between Water and Cement (Figure 3, Point #2)

Once infiltrating water that is equilibrated with alluvial soils encounters the vault, it will react with a large mass of reinforced concrete, altering the solution composition. These changes in solution composition can be modeled using either kinetic or thermodynamic approaches if the composition of concrete is known. This study will model concrete and cement impacts using chemical thermodynamics.

Reinforced concrete consists of hydrated cement aggregate supported by an internal super-structure of steel rods. The size, composition, and distribution of the steel bars are designated based on performance criteria. Cement aggregate is a hydrated mix of minerals that forms when dry Portland cement feedstock reacts with water and filler materials to create a solid aggregate product. The main components of the dry Portland cement feedstock used to synthesize cement aggregate are summarized in Table 4.

When the dry feedstock components of the Portland cement and filler materials are mixed with water, they react to form a new mixture of hydrated minerals that is geochemically distinct from dry Portland cement. The mineral mixture formed is variable, but typically contains 20 to 25% portlandite ($CaOH_2$), 40 to 50% amorphous CSH gel, 10 to 20% iron and aluminum oxides, 10 to 20% pore solution, and 0 to 5% minor components (e.g., KOH, $Mg(OH)_2$, and NaOH) (Alexeev 2001). The composition can be manipulated to achieve desired structural characteristics or chemical properties.

Table 4. Primary components of dry Portland cement feedstock (Mindess and Young 1981).

| Chemical Name | Chemical Formula | Shorthand Notation | Percent by Weight |
|---|---|---|---|
| Tricalcium silicate | $3CaO{\cdot}SiO_2$ | $C_3S$ | 50 |
| Dicalcium silicate | $2CaO{\cdot}SiO_2$ | $C_2S$ | 25 |
| Tricalcium aluminate | $3CaO{\cdot}Al_2O_3$ | $C_3A$ | 12 |
| Tetracalcium aluminoferrite | $4CaO{\cdot}Al_2O_3{\cdot}Fe_2O_3$ | $C_4AF$ | 8 |
| Gypsum | $CaSO_4{\cdot}H_2O$ | $CSH_2$ | 3.5 |

Equilibrium, batch-mode thermodynamic calculations conducted by Berner (1992) indicate that cement dissolution will slowly release aqueous $H_XSiO_3$, Ca, and $OH^-$ ions into solution; and that the equilibrium state of the system varies over time with the Ca/Si ratio of the cement. Results from Berner's calculations (Figure 5) indicate that when the Ca/Si ratio of the cement is less than 0.9, solution pH ranges from 7.5 to 10.5 and total aqueous calcium (Ca-aq) is less than 2 mmol/L. As the cement becomes more

Ca-rich, pH increases and Ca-aq in groundwater rises rapidly to a maximum of 20 to 22 mmol/L. Berner's calculations are generally consistent with results from experimental studies involving continuous flow experiments in saturated systems (Dayal and Readson 1992, Toyohara et al. 2000, Fuhrman and Gillow 2009), Appendix B of Krupka and Serne (1998), and field studies of natural analogues (McKinley and Alexander 1992).

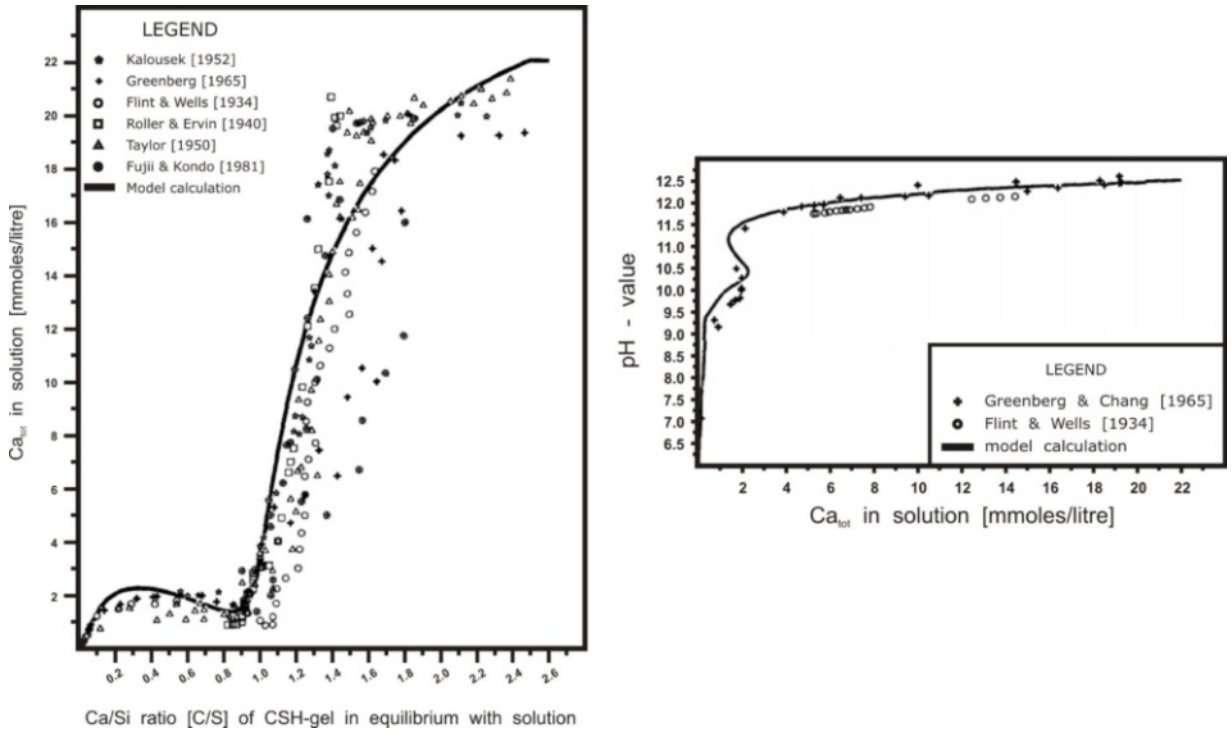


Figure 5. Composition of water in equilibrium with mature cement in a closed system and impact of Ca/Si ratio (Ca-aq in left figure and pH in right figure from Berner [1992]).

### 2.4.1 Conceptual Model for Cement Degradation

Berner's cement model provides a reasonable basis for calculating the impacts of cement dissolution on solution composition. His publications provide thermodynamic parameters that accommodate a range of Ca/Si ratios, a mass composition of a "typical" cement aggregate, and descriptions of how dissolution of that aggregate alters solution composition over time. Adopting Berner's description facilitates development of a cement model that can estimate solution composition as cement ages. For batch-mode calculations, Berner's model can be applied to the following three cement scenarios:

1. *Fresh cement* – Equilibrium with cement where NaOH and KOH are still present and control solution chemistry (pH about 13 to 14).
2. *Mature cement* – Equilibrium with cement where NaOH and KOH have been leached out and solution chemistry is controlled by portlandite (pH about 11 to 13).
3. *Degraded cement* – Equilibrium with cement where NaOH, KOH, and portlandite have leached out and solution chemistry is controlled by CSH gel with varying Ca/Si ratio (pH about 9 to 11).

In addition to the fresh-to-degraded cement chemical progression described by the batch model of Berner, the resultant chemical modifications alter physical properties of cement. An instructive example is provided by Fujiwara et al. (1992), who analyzed the physical and chemical composition of a 60-year old concrete revetment emplaced within soft, muddy ground. Their results indicate that the reaction of cement with soil water alters the physical structure and geochemical composition of the cement in a

manner that varies with the distance from the outer cement surface into the cement revetment. According to their observations, cement degradation (1) increases pore size and volume for regions closer to the water-cement interface, (2) decreases the ratio of calcium oxides to insoluble minerals for regions closer to the water-cement interface, and (3) decreases pH for solution in contact with areas of the cement closer to the water-cement interface. Their solution and solids characteristics are summarized in Table 5 as a function of distance from the surface of the concrete revetment.

Table 5. Potential impact of cement-water interactions on mineral and solution chemistry at the water-cement interface (from Fujiwara et al. 1992).

| | Solution pH | Ca/Si Ratio | CaO Minerals/ Insoluble Minerals | Percent Calcite | Percent CSH |
|---|---|---|---|---|---|
| Surface | 9–11 | 0.25 | 0.05–0.1 | 25–55 | 25–60 |
| Interior | 11.0 | 0.75 | 0.12 | 5 | 65 |
| Percent Change | 9% | 67% | 33% | 500% | 23% |

These data show the solution pH increasing from the surface toward the interior, with corresponding cement mineral composition consistent with the general trends shown in Figure 4. Across all samples, the Ca/Si ratio at the surface reached a minimum of about 0.25, regardless of the ratio in the interior. This change corresponded with fewer calcium oxide minerals relative to insoluble silicon oxide minerals, a reduced mass percent of CSH gel, and an increased mass percent of calcite at the surface. The soil and water conditions expected at the RH-LLW disposal facility location are expected to be similar to those encountered at other vault locations across the INL (i.e., Active Low-Level Waste Disposal Facility at the RWMC). These vaults have experienced no significant general degradation or development of fissures in the 20+ years they have been installed. However, the facility must perform as designed through at least 500 years, and the degraded cement of Fujiwara et al (1992) can be used as an indicator of the long-term degraded state of the RH-LLW disposal facility vaults.

The evolution of pore water composition as it slowly degrades cement surfaces will be complicated by the components of the RH-LLW vault system as discussed previously, and development of a comprehensive model that accounts for all changes is beyond the scope of this work. However, both Berner (1992) and Reardon (1992) demonstrate that a reasonable approximation of potential cement impacts on solution chemistry can be achieved with a relatively simple equilibrium model. The difficulty in constructing such a model lies in developing an internally consistent thermodynamic dataset from multiple sources and in accurately specifying the composition of the cement, including minor phases. This study adopts the thermodynamic constants and hydrated Portland cement system as described by Berner (1992). Berner treats cement as a mixture of amorphous silicon oxides, portlandite, and CSH-gel in a solid solution, with the dissolution coefficients for these mineral species dependent on the Ca/Si ratio of cement. All other components have thermodynamic coefficients that are independent of cement composition. Adopting Berner's cement description allows the development of a model that describes solution composition over a broader range of Ca/Si ratios than other published approaches, and will allow the same thermodynamic dataset to be used to model cement interaction with infiltrating water as cement ages (e.g., fresh, mature, or degraded). The composition for fresh cement used in model calculations is given in Column 3 of Table 6.

Replicating Berner's model results for mature cement (Figure 5) requires excluding hydrogarnet, ettringite ($AF_t$), and monosulfate ($AF_m$) from the system. Therefore, fresh cement is defined as the components given in Column 3 of Table 6, minus these phases and using a Ca/Si ratio of 1.8. Mature cement is defined as fresh cement, minus the NaOH and KOH components. Degraded cement is defined as cement where solution pH is controlled by a mixture of calcite and CSH gel, with a minimum Ca/Si ratio. This ratio is assumed to be 0.25, based on the work of Fujiwara et al. (1992). The changes in mineral composition as cement degrades are approximated by the difference between the surface and

interior assemblages described by Fujiwara et al. (Table 5). The model for degraded cement assumes that cement degradation replaces all portlandite with calcite and that 25% of all CSH gel is replaced by a mixture of amorphous silica ($SiO_2$-am) and calcite. All remaining CSH gel has a Ca/Si ratio of 0.25. Also for degraded cement, the dissolution coefficient for $SiO_2$-am is as defined by Berner (1992) for a Ca/Si ratio less than 1.

Table 6. Cement composition for two variants of hydrated Portland cement (from Berner 1992). The solid solutions are mixtures of portlandite and Ca-Si-hydrate.

| Model Components | Hydrated Portland Cement/Trass Mixture mmoles/kg of Hydrated Mixture | Hydrated Sulphate-Resistant Portland Cement mmoles/kg of Hydrated Cement |
|---|---|---|
| *$C_3S_{0.725}F_{0.275}H_6$ (solid sol) | 401 | |
| *$C_3A_{0.17}F_{0.83}H_6$ (hydrogarnet, solid sol) | | 384 |
| *$C_6AS_3H_{32}$ (ettringite or $AF_t$) | | 16.1 |
| *$C_4ASH_{12}$ (monosulfate or $AF_m$) | 146 | 192 |
| $C_{1.39}SH_{1.39}$ | 3,620 | |
| $C_{1.8}SH_{1.8}$ (CSH) | | 2,386 |
| CH (portlandite) | | 1,420 |
| MH (brucite) | 144 | 208 |
| KOH | 196 | 148 |
| NaOH | 97.2 | 22.4 |
| $CaCO_3$ | 31.5 | |
| Free water | 7,211 | 5,560 |
| Estimated density | 2,030 kg/m$^3$ | 2,090 kg/m$^3$ |
| Estimated total porosity | 26% | 21% |

* Not considered in the thermodynamic cement model of Berner (1992).

Note that, because hydrogarnet, ettringite ($AF_t$), and monosulfate ($AF_m$) are excluded from the system, this model does not consider the impacts of ettringite and monosulfate dissolution and precipitation on solution composition. In reality, these reactions will alter solution chemistry and radionuclide sorption dynamically along transport paths. However, they represent a small fraction of the mass composition of hydrated cement, and their impacts on solution composition are anticipated to be relatively minor compared to the effects of portlandite and CSH. Accurately modeling their secondary impacts would require a larger modeling effort, validating data, and a more comprehensive cement thermodynamic dataset. The simple model is sufficient to the needs of this project, which is to estimate the likely boundaries of solution composition so that bounding estimates of minimum $K_d$ values can be made from the basis of site-specific studies and literature reports.

### 2.4.2 Calculation of the Composition of Infiltrating Water Reacting with Cement

In the following calculations, it is assumed that water will primarily infiltrate into the vault through cracks in the cement that form after the engineered cap is put into place. This assumption is based on the work of Walton and Seitz (1992), who provide a detailed analysis of fluid flow through fractures in underground concrete vaults. Their work suggests that water pools on top of concrete vaults, leading to saturated flow that preferentially moves through middle-sized cracks (i.e., about 0.05 to 0.1-mm width). The rate of flow into the cracks is impacted by the permeability of the overlying soil, and flow is greatest when cracks are narrowly spaced (i.e., 1 to 10% of cement volume). To provide a bounding estimate emulative of maximum infiltration scenarios, we have assumed that saturated flow occurs through cement with 10% additional porosity to account for potential cracking. This yields a total porosity of 31% if it is

further assumed that native porosity and cracks are hydraulically connected. Cement properties are otherwise as described in Column 3 of Table 7. At 31% porosity, there are 3.2 $m^3$ of cement per cubic meter of aqueous solution or 6.69 kg Portland cement per kg solution. The geochemical model is formulated on the basis of kilograms aqueous solution, thus the mass of cement constituents listed in Table 6 (Column 3) is multiplied by 6.69 when defining the molar composition of cement that can react with 1.0 kilogram of infiltrating water.

Table 7. Composition of INL alluvium water in equilibrium with fresh, mature, and degraded cement under a soil gas atmosphere. Range represents difference between minimum salinity and maximum salinity per Table 2. Water corresponds to what is anticipated to occur at Point #2 in Figure 3.

| Parameter | pH | Ca-aq (mM) | Mg-aq (mM) | Na-aq (mM) | K-aq (mM) | ΣCO2-aq (mM) | Cl-aq (mM) | SO4-aq (mM) | NO3-aq (mM) | OH- (mM) | Si-aq (mM) | Ionic strength (mM) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Fresh (Ca/Si = 1.8) | 14.1 | <0.1 | <0.1 | 145–160 | ~950 | ~16 | 0–7.5 | 0.3–7.3 | 0–7.8 | ~800 | ~35 | 940–970 |
| Mature (Ca/Si = 1.5) | 12.3 | 7–12 | <0.1 | 1.2–17 | 0–2 | <0.1 | 0–7.5 | 0.3-7.3 | 0–7.8 | ~12 | <0.1 | 20–50 |
| Degraded (Ca/Si = 0.25) | 10.3 | 1.3–6 | 0.2–0.8 | 1.2–17 | 0–2 | <0.1 | 0–7.5 | 0.3–7.3 | 0–7.8 | 0.1–1.2 | ~5 | 6–40 |

To determine the water chemistries provided in Table 7, cement-water systems corresponding to fresh, mature, and degraded cements were modeled in batch mode using PHREEQc (v 2.17), which is a standard geochemical model developed by the U.S. Geological Survey. The calculations were conducted on the cement mineral system for mature cement paste as described by Reardon (1992; Tables 7 and 8), using the "llnl.dat" thermodynamic database modified to include cement reactions as described by the model of Berner (1992). Charge balance is not forced in this approach; however, charge-balance errors are typically less than 5 to 10%. The thermodynamic expressions presented by Berner have been recalculated so that they are consistent with the reactive components used by PHREEQc; the expressions are provided in Appendix A. This primarily involved rewriting reactions (and recalculating coefficients) to replace $OH^-$ with $H_2O$ and $H_2SiO_4^{2-}$ with $SiO_2$-aq; and balancing reactions as needed. Berner did not provide all thermodynamic data needed to model fresh cement with his approach. In these cases, dissolution coefficients are either as reported by Reardon (1992), as possible, or Lothenbach and Winnefeld (2006). Lothenbach and Winnefeld (2006) have compiled the most extensive dataset available on the thermodynamics of cement components. However, their dataset does not account for the chemistry of solid solutions of portlandite and CSH gel over the range of Ca/Si ratios described by Berner (1992).

The ideal modeling approach would be to combine the solid solution dataset of Berner with the comprehensive dataset of other cement components provided by Lothenbach and Winnefeld (2006) and then use that new dataset in a dual-porosity reactive transport calculation. Doing this would require that the solid solution coefficients, as reported by Berner (1992), be derived again using the more comprehensive dataset for cement provided by Lothenbach and Winnefeld (2006) and then using the dataset of Lothenbach and Winnefeld for all calculations. It would also require gathering hydrologic parameters and conducting sensitivity studies for reactive transport simulations. However, the composition and physical properties of the cement to be used at the RH-LLW facility is not yet known. Therefore, the precision gained from doing these additional calculations is believed to be less than the uncertainty associated with time-variable cement properties. Consequently, the significant effort required to do this series of calculations currently is not justifiable. Given current knowledge, augmenting the internally consistent dataset of Berner with additional coefficients for minor constituents is sufficient for the project objectives.

Results from model calculations using the range of solution chemistry from Table 2 (minimum and maximum) are presented in Table 7 for fresh, mature, and degraded cement. The model predictions are

within the pH and aqueous calcium (Ca-aq) ranges reported by previous researchers (e.g., Figure 5), though the concentration of Ca-aq is at the lower end of prior reports. The cause of this discrepancy has not been evaluated in detail. One cause could come from the method in which ionic strength is used to determine the chemical activities of reactive constituents. If activity coefficients are overestimated, then aqueous concentrations will be underestimated. Other possibilities could be that the combination of thermodynamic data from multiple datasets leads to internal inconsistencies that generate errors or in the way that gaseous $CO_2$ is treated. Also, $SO_4^{2-}$ predictions would be different if sulfate-containing cement minerals (e.g., ettringite and monosulfate) were included in the calculations. Such errors could be reduced by building an improved thermodynamic dataset and running additional sensitivity studies.

The 1,000 year compliance period for the RH-LLW disposal facility and inherent variation in groundwater chemistry during the three stages of cement degradation raises the question of which scenario provides the most appropriate estimate of conditions in the RH-LLW facility. Berner (1992) used a simple batch-equilibrium and solution exchange model to estimate that KOH and NaOH would leach out within 100 water exchange cycles, while portlandite would persist for over 7,500 exchange cycles. Jacques et al. (2010) have estimated that NaOH and KOH are leached within the first 0.5 kg of water per liter of cement, while portlandite persists for about 75 kg water per liter cement. Infiltration rates into the vault at the RH-LLW facility will be extremely slow, and only 6 to 80 total pore volumes of water (e.g., both sand infill and cement) are expected to pass through the vault system during the first 1,000 years under baseline conditions (~180 pore volumes in catastrophic failure scenarios). Approximately 7 times more water is estimated to move through sand infill than through cement. This would suggest that fresh cement would persist and influence the pore water chemistry within the vault during the compliance period. However, the data collected by Fujiwara et al. (1992) suggests cement degrades in layers, with the outermost layer more degraded than the inner layers. Therefore, it is possible that a thin layer of mature or degraded cement may control solution chemistry within the first 1,000 years, even though bulk composition batch calculations might indicate that fresh cement would be expected to control solution chemistry. This problem cannot be fully resolved without a more comprehensive evaluation of long-term cement performance under conditions similar to those expected at the RH-LLW disposal facility concurrent with modeling using cement with the same composition expected to be used in the RH-LLW vault. Such work is beyond the scope of this bounding study. *Given the inherent uncertainty, subsequent calculations will be performed for both water in contact with fresh cement and water in contact with mature cement. These two cement compositions are considered to provide reasonable bounds for water composition within the vault interior*.

The considerations discussed in this section have neglected the presence of steel rebar in the reinforced cement. Interaction of infiltrating pore water with cement rebar will alter solution chemistry for water that infiltrates into the vault, but not water that remains outside the vault. The impacts of cement rebar and corrosion of steel waste liners are assessed in the following subsection for both fresh and mature cement.

## 2.5 Evaluation of Chemical Reactions between Water, Concrete Rebar, and Corroding Steel Liners (Figure 3, Point #3)

Cement contains iron rebar that can corrode and alter solution composition as water infiltrates through concrete. Further, after the infiltrating alluvium water has interacted with cement, it will accumulate on steel liners, corrode them, and then infiltrate through the container into the waste package. During this sequence of events, the water infiltrating through the top of the cement vault may mix with water that has condensed on vault surfaces (from soil moisture) or was enclosed within the steel liner along with the waste resins or metallic reactor parts. These calculations assume that condensate will contribute only a small proportion of the total mass of water that will contact the waste over time. Therefore, condensate should not significantly alter the composition of solutions in the vault environment.

### 2.5.1 Conceptual Model of Metal Corrosion

Metal corrosion in aqueous systems is an oxidative, acid-generating process that consumes $O_2$ during oxidation of zero-valent metals in the steel alloy, and then produces $H^+$ atoms during the subsequent precipitation of the metal oxide minerals that are the main product of corrosion reactions. Resulting changes in pH and oxidation state of the infiltrating solution are dependent on the rate of corrosion. These changes could impact the major ion composition of the solution, and the $K_d$ of contaminant release and sorption in the vault. Most available information on steel corrosion in cementitious environments comes from studies of the durability of reinforced concrete. The high pH of the cement environment inhibits corrosion, with the degree of inhibition dependent on pH, aqueous chloride, and steel type. Elevated $Cl^-$ levels stimulate corrosion, but the high pH of concrete environments inhibits corrosion by favoring precipitation of passivating layers of iron oxides (Kouril et al. 2010, Gu et al. 1996, Hartt et al. 2004).

The steel liners will likely be made of either carbon steel or stainless steel. The metal waste components are predominantly stainless steel, Zircaloy, and Inconel, which are notably more resistant to corrosion than carbon steel. The approximate compositions of carbon and stainless steels are as follows:

- *Carbon steel* – 98% Fe and less than 2% other (C, Mn, P, S, Cr, Cu, Ni, Mn, and Mo)
- *Stainless steel* – 65% Fe, 20% Cr, 10% Ni, and less than 2% other (C, Mn, Mo, Cu, Si, and Ti).

Chromium and nickel in stainless steel inhibit corrosion (Kouril et al. 2010), but have been observed to be lost from the corroded steel in approximate proportion to their proportion of mass composition (Kadry 2008). Their subsequent fate will be dependent on sorption and precipitation reactions that are controlled by solution chemistry. It is highly unlikely that chromium and nickel in stainless steel would elevate the levels of these non-radioactive constituents above environmental risk thresholds. The mass of stainless steel corroded is likely to be small in the dry environment of the vault, and most metals released should precipitate as oxyhydroxides. Thus, the impact of chromium release due to stainless steel corrosion is considered to be inconsequential with respect to the analysis of $K_d$. This analysis assumes that the only impacts of corrosion on solution chemistry are a reduction in pH and oxidation state (pe).

At high pH, chloride is known to enhance corrosion rates at aqueous concentrations above 30 mmol per liter for stainless steel (Kouril et al. 2010), and above 4 to 8 mmol per liter for carbon steel (Li and Sagüés 1999). INL alluvium water has a median concentration of 1.0 mmol per liter, with a maximum observed concentration of 7.5 mmol per liter. This is below the concentrations at which chloride enhances corrosion of stainless steel at high pH; and at the threshold for which chloride enhances corrosion of carbon steel. Consequently, chloride infiltration is not likely to impact steel corrosion rates in the RH-LLW vault environment *as long as the cement materials used to construct the vault have low chloride content and chloride salts are not otherwise added to the system.*

Exposure to temperatures in excess of 550°C for periods of greater than 10 to 12 hours can lead to the formation of chromium carbide precipitates that concentrate chromium in specific spots, while also creating physical stresses in the steel. These changes disrupt the ability of chromium oxide coatings to inhibit corrosion and accelerate the rate of stainless steel corrosion. This process is known as sensitization. This study will address this issue by estimating the chemical impact of corrosion for both stainless steel and carbon steel. For conservatism, sensitized stainless steel is assumed to corrode at the same rate as carbon steel, and carbon steel is assumed to provide a bounding scenario that estimates the maximum potential impact of steel corrosion on solution chemistry and resin $K_d$. This also assumes Inconel and Zircaloy corrode at the rate of carbon steel. The assumption allows more corrosion products to be in aqueous solution than would occur in the RH-LLW disposal facility.

Corrosion will be modeled using a hybrid kinetic/thermodynamice approach. All iron that undergoes a corrosion reaction is assumed to react to equilibrium, but the mass of iron that reacts is kinetically determined for each infiltration case. The same numerical approach will be taken for each type of steel, with only the rate constants varying. This study will evaluate the chemical impact of corrosion on

infiltrating solutions by estimating how much iron and acidity is released into solution by corrosion processes during the residence time of water in the vault interior. We also assume that any acidity will be neutralized by the vault floor before exiting to the underlying alluvium.

### 2.5.2 Calculation of the Composition of Infiltrating Water Reacting with Reinforced Cement and Steel Waste Liners

The potential impact of steel rebar corrosion on solution chemistry in the RH-LLW vault has been assessed via geochemical modeling analogous to that described in Section 2.3, with the difference being that these calculations evaluate reinforced cement (e.g., cement plus rebar). The calculations assume that, by mass, 12.5% of the reinforced concrete is steel. This estimate comes from comparing the density of hydrated Portland cement from Table 6 with the typical density of reinforced concrete, which is 2,400 kg per $m^3$. Based on this comparison, reinforced concrete that is 12.5% rebar by mass would contain 2,090 kg per $m^3$ concrete and 310 kg per $m^3$ of steel rebar. Steel corrosion is modeled using data for steel corrosion in INL alluvium water as reported by Adler-Flitton et al. (2004, 2011). For bounding purposes, this calculation assumes that bare mild carbon steel is used for rebar and adopts the average corrosion rates reported by Adler-Flitton et al. (2004, 2011) for mild carbon steel corrosion at near-neutral pH. The actual corrosion rates are likely to be much lower because steel corrodes much more slowly in a cementitious environment (high pH) than at near-neutral pH (Kouril et al. 2010, Gu et al. 1996, Hartt et al. 2004, ACI Committee 222 2001). This assumption will likely overestimate the impact of steel rebar corrosion on solution chemistry. In the absence of high chloride levels, carbon steel will corrode very slowly in the high-pH cement environment. Thus, by assuming that steel will corrode at the much greater rate observed in soil pH environments (e.g., pH 6 to 8), we are assuming a chemical impact much greater than would occur under all anticipated scenarios.

The impact of steel liner corrosion on solution chemistry in the RH-LLW vault is assessed by reacting cement-equilibrated water with uncoated carbon steel not in contact with cement. This assumption likely overestimates total corrosion, as some containers will be made of stainless steel (e.g., NRF resins). For this calculation, the Naval Reactors Facility (NRF) section is assumed to be emulative of the overall RH-LLW facility. The total mass of steel waste liners to be placed within the NRF section of the RH-LLW facility is currently estimated to be 573,864 kg in 240,000 $ft^3$ of storage space (A. J. Sondrup, personal communication, July 29, 2010). This equates to an effective steel density of approximately 85.4 kg steel per cubic meter of vault space, or approximately 1.0 to 1.5 moles iron per liter vault space, depending on steel type. The kinetic expressions for steel corrosion developed by Adler-Flitton et al. (2004, 2011) for corrosion of steel coupons in INL alluvial sediment were selected for over the rates determined in the CPP-749 (INL 2009) air environment because corrosion of carbon steel in soil occurs at a faster rate than corrosion in air. Additional differences between the buried coupon studies of Adler-Flitton et al. (2004, 2011) and the RH-LLW disposal facility vault environment, enumerated below, should cause the steel corrosion rates in the vault to be lower than those measured in INL alluvium soils.

- Adler-Flitton et al. (2004, 2011) reported the presence of soil microbes on the coupons that could enhance corrosion rates. The steel liners are not in contact with soil and lack the organic matter and nutrients found in soil systems. This will inhibit microbially catalyzed corrosion processes.
- Water that condenses on steel liners will have a lower pH than soil water (due to a lack of carbonate minerals). However, most of the water that encounters the liners will likely come from drips that originate on the ceiling of the cement vault, either from infiltration through cracks in the cement or soil moisture that condenses on the cool cement (cement will be cooler than the liners because radioactive decay will warm the liners more than the cement). This water will have reacted with cement minerals and have an elevated pH. Steel corrosion at the high pH found in cement environments is typically 100 to 1,000 times slower than at neutral pH (Kouril et al. 2010, Gu et al. 1996, Hartt et al. 2004, ACI Committee 222 2001). Therefore, the presence of cement-leachate source water will lower corrosion rates below what they would be in soil water.

- The soil coupons used by Adler-Flitton et al. (2004, 2011) did not contain mixtures of metals that could form galvanic cells, which accelerate corrosion rates for the anodic material. However, the data reported in INL 2009 showed minimal differences in corrosion of stainless steel components in contact with aluminum and carbon steel. The steel liners will contain mixtures of metals and the drain valves are a different metal than the container walls. Most of the metals used are more cathodic than carbon steel; therefore, the rate of corrosion of carbon steel could be accelerated through the formation of galvanic cells. However, this acceleration is offset by two mitigating factors: (1) many of the carbon steel liners have an epoxy coating on the inside that prevents metal-to-metal contact and protects the internal surfaces from galvanic corrosion and (2) corrosion requires wetted contact to move ions from the cathodic metal to the anodic metal. In an unsaturated environment, extensive wetted contact will likely only occur in crevices and locations where two liners are in contact with each other. This will limit the area of galvanically enhanced corrosion and reduce the overall impact of galvanic corrosion on solution chemistry.
- Pillay (1986a) reports that radiation can enhance the rate of degradation of ion-exchange resins made from synthetic organic materials when such resins are wet or moist (as is the case in the waste liners). The degradation products of this radiolysis are corrosive and have been reported to enhance the corrosion rates of carbon steel. However, resins will not be present in all liners, radiolytic impacts will decline over time with declining dose rate, and the internal epoxy coating of the carbon steel liners will slow corrosion. Furthermore, this corrosion enhancement should be minor for all cases where resin containers are stored with other resin containers (e.g., lower radioactive flux).

The combination of these factors makes it unlikely that corrosion rates for carbon steel observed within the vault would exceed those measured by Adler-Flitton et al. (2004, 2011) for corrosion in INL alluvium soils. Corrosion rates for all activated metal components should be orders of magnitude slower than those reported for carbon steel (Adler Flitton et al. 2004, 2011, and Adler Flitton and Yoder 2009). Thus, utilization of the Adler-Flitton data provides a reasonable basis for bounding calculations. The liner corrosion model also specifies that solution is no longer in contact with concrete, excluding cement minerals from the calculations. Dissolution/precipitation reactions involving calcite, goethite, amorphous iron hydroxide, portlandite, and amorphous $SiO_2$ are assumed to moderate solution composition.

As with non-reinforced concrete, a simplified PHREEQc model was used to conduct all geochemical calculations. Charge balance was not forced, but charge-balance errors were less than 5 to 10%. The initial solution was assumed to be under a constant partial pressure of 0.18 atm $O_2$ within the cement pore spaces and while in contact with the steel liners in the vault. $O_2$ is depleted through chemical reactions. The only electron donor is the zero-valent iron in the cement rebar and steel liners. Oxygen, $NO_3^-$, $SO_4^{2-}$, and aqueous carbonate species are the electron acceptors, with $O_2$ being consumed first. The oxidation state of the system can vary as a function of the degree of steel corrosion, with more steel corrosion correlating to less oxygen and a more reducing system. However, the system will be in equilibrium with soil gas that contains $O_2$ and it is assumed that the bulk solution will always contain $O_2$.

Data reported by Adler-Flitton et al. (2004, 2011) for corrosion of carbon steel in a soil environment is provided in Figure 6 for two soil depths. These data indicate that corrosion is a non-linear process, where corrosion rates decrease logarithmically over time according to a first order rate law. Results in Figure 6 are plotted as mass loss from the steel coupon rather than the actual mass of steel remaining in the coupon; therefore, they plot as the inverse of the exponential function that describes a first order reaction rate (e.g., ln(x) rather than $e^x$). Two different rate relationships are observed, with steel that is buried deeper corroding more quickly. Soil moisture is typically higher at deeper depth in INL sediment, and the higher corrosion rates at a 10-ft depth may be associated with greater soil moisture content. This higher corrosion rate will be adopted for these bounding studies (e.g., grams of steel lost per 150 grams of carbon steel = 2.05 * ln(time in years) + 0.88).

This corrosion rate was measured for rectangular coupons that were 3 x 3 x 1/8-in. with a 0.56-in.-diameter hole in the center. Total mass loss is proportional to both the surface area to volume ratio of the coupon and the amount of steel present. Each coupon weighed approximately 150 grams. If it is assumed that differences in the surface area to volume ratio between the coupons and the waste containers is of secondary importance in estimating maximum likely corrosion rates in the RH-LLW vault, then the corrosion data of Adler-Flitton et al. (2006, 2011) can be used to bound the impact of corrosion on the chemistry of solutions that come into contact with the resins. Under this assumption, if the higher mass loss rate from Figure 6 is applied to the water residence time scenarios previously presented (e.g., Section 2.3), then each liter of water will be exposed to corroding steel for 3 to 350 years and corrosion rates will range from 3 to 13 grams steel lost per 150 grams of carbon steel (e.g., 20 to 87 grams steel lost per kilogram steel) for the respective time period. For each infiltration scenario, the total rates of steel loss depend on the kilograms of steel present per kilogram of total volume that water encounters (e.g., the system also contains concrete and empty space). The total mass of steel that each kilogram of water encounters as it transits the system is estimated as follows:

- *For carbon steel in concrete rebar:* Calculations are based on values in Table 6 for cement and are adjusted for steel rebar in reinforced concrete:
  - 2,090 kg Portland cement plus 310 kg carbon steel per cubic meter of reinforced concrete.
  - 31% porosity for cement (21% native cement porosity + 10% from cracks), with native pores hydraulically connected to cracks. For the purposes of this bounding batch calculation, it is assumed that all cement and rebar can come into contact with infiltrating water.
  - From porosity, there are 3.2 $m^3$ of reinforced concrete per cubic meter of aqueous solution. This equates to 6.690 kg of Portland cement and 0.99 kg carbon steel per kg of aqueous solution.
- *For carbon steel waste containers:* Current plans are for all waste containers, except those containing NRF resins, to be carbon steel. For this calculation, it will be assumed that all containers are made of carbon steel and corrosion proceeds more quickly than should occur in the real system. Calculations are based on water that has fully reacted with carbon steel in cement and is in equilibrium with Portland cement before leaving the cement environment and corroding carbon steel waste containers.
  - Current planning assumptions indicate that there will be 85.4 kg of steel in containers per cubic meter of vault space. .
  - Assume a maximum of 10% of total vault space contains water. This equates to 100 L of solution per cubic meter of vault space.
  - From above, 100 L of solution will encounter 85.4 kg of steel in carbon steel containers. This equates to 0.85 kg carbon steel per kg of aqueous solution.
- *Gas phase composition:* The reactions described above consume oxygen and produce acidity that can alter solution chemistry in both environments (e.g., cement-rebar and steel liners). The gaseous composition is specified separately for the two environments:
  - *For cement-rebar*: This system is assumed to consist of saturated flow of solution that is in contact with a large volume of soil gas. In PHREEQc, it is modeled with a constant pressure gas phase with a 1,000-L gas volume. Soil gas is assumed to be oxic, with elevated $pCO_2$. By pressure, the gas is 80% $N_2$, 18% $O_2$, and 2% $CO_2$. $N_2$ is assumed to be chemically inert.
  - *For steel containers in the vault-interior:* Because of the saturated state of the water in the overlying cement, the vault is assumed to be isolated from the soil gas above it and to the sides. However, the vault will have perforations in the bottom to allow drainage. These perforations will keep the vault in atmospheric contact with soil gas from the vault underlayment and RH-LLW alluvium. In PHREEQc, this is treated as a separate constant-pressure gas phase with the same gaseous composition and volume as for the cement rebar case.

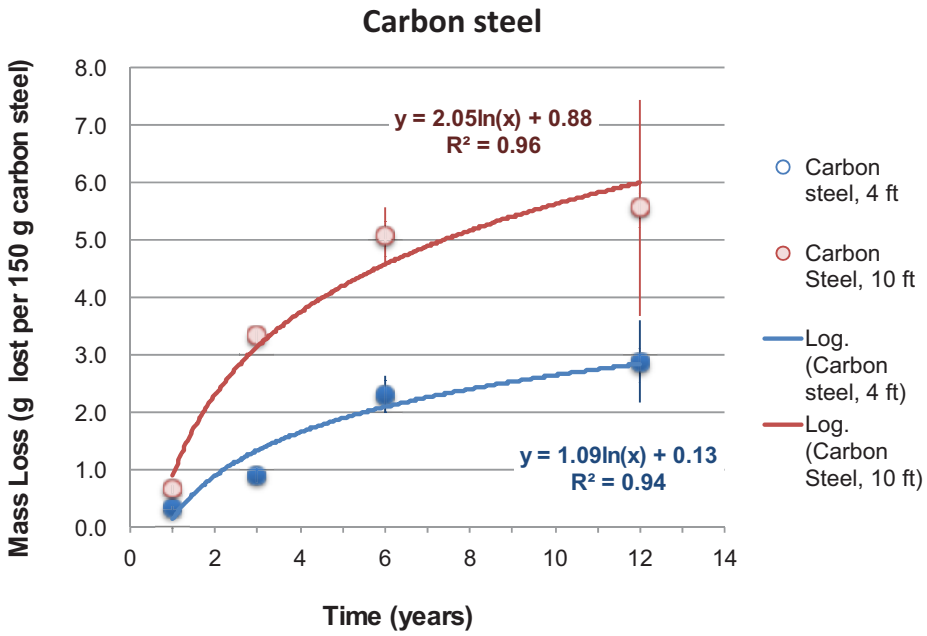


Figure 6. Results of corrosion tests conducted by Adler-Flitton (2004, 2011). Plotted data are the average and standard deviation of 4 coupons. Measured mass loss is proportional to total mass present.

Model calculations emulate the Adler-Flitton et al. (2004, 2011) corrosion reaction rates by equilibrating a specified total mass of zero-valent iron with the infiltrating water over 50 to 100 equal time steps. For 100 time steps, this equates to 3 years per step for a 300-year residence time and 0.03 years per step for a 3-year residence time. PHREEQc requires inputs of total mass added and number of time steps. The number of time steps is a numerical parameter to facilitate model convergence and does not significantly alter model predictions. The total mass of iron added per kilogram water over the residence time of water in the vault system (e.g., cement cap plus vault interior) for each combination of infiltration and corrosion scenario are summarized in Table 8.

Table 8. Mass of iron that reacts with each kilogram of infiltrating water over the residence time of a kilogram of water (median value) in the vault systems for various infiltration and corrosion scenarios. Calculations assume that grams of iron = 0.98 * grams of carbon steel and 55.85 grams iron per mole. Total moles corroded are calculated based on the median residence time.

| Infiltration Scenario | Residence Time (years) | Pore Volumes per 500 Years | Total mol Fe Corroded per kg Solution (rebar) | Total mol Fe Corroded per kg Solution (liners) |
|---|---|---|---|---|
| 0 to 500 years, baseline | 300 | <2 | 1.5 | 1.3 |
| 0 to 500 years, failure | 3 to 18 (median = 10) | 30 to 190 | 0.4 | 0.3 |
| 500 to 1,000 years, baseline | 150 to 200 (median = 175) | 2 to 4 | 1.3 | 1.1 |
| 500 to 1,000 years, failure | 60 to 100 (median = 80) | 4 to 8 | 1.1 | 1.0 |
| >1,000 years | 180 to 330 (median = 255) | 3 to 6 | 1.4 | 1.2 |

Corrosion estimates in Table 8 provide for three general scenarios of iron corrosion in rebar and steel containers. Each of these scenarios breaks the total corrosion impacts within the vault system into two

steps: vault plug (e.g., concrete rebar) and steel liners. The calculations assume non-linear corrosion and that the relatively short-term corrosion rates observed for Adler-Flitton et al. apply over time periods in excess of 100 years. The impact of corrosion on solution chemistry increases with increasing water residence time, but the impact is small. For fast transit with water residence times of less than 20 years, less than 1.0 mol of iron is corroded per kilogram of solution while within the vault zone. For longer transit times, 2 to 3 moles of iron are corroded per kilogram of infiltrating solution. The model calculations separately consider the impacts of corrosion in concrete rebar and steel liners, even though the residence time is calculated for the overall vault system. This is done because the presence of cement buffers the pH impacts of rebar corrosion, but does not buffer the pH impacts of liner corrosion.

The greatest impacts on solution chemistry come from cases with long residence times (more opportunity for corrosion). Model calculations for the 0 to 500-year baseline infiltration scenario with a 300-year residence time yield the greatest impact on solution chemistry. Data for this scenario are provided in Table 9 and indicate that rebar in cement does not measurably alter solution chemistry for either fresh or mature cement. The calculations indicate that, over a 300-year vault transit period, corrosion of carbon steel in rebar can potentially consume up to 1.1 moles of $O_2$ per liter of water in contact with steel. This maximum-possible value is roughly equivalent to stripping all the $O_2$ from approximately 0.5 L of soil gas per liter of aqueous solution per year at standard temperature and pressure. In practice, corrosion rates for bare carbon steel in contact with solution at near-neutral pH greatly overestimate corrosion of steel in concrete rebar. Steel corrosion in concrete environments will be inhibited by the high pH of the cement-leachate solution and steel will likely be cladded to inhibit corrosion. The combination of these two factors would be anticipated to reduce corrosion by a factor of about 1,000 (Hartt et al. 2004, ACI Committee 222 2001). At this inhibited rate, corrosion would strip all $O_2$ out of less than 0.001 L of soil gas per year. Given typical rates of soil-gas exchange and anticipated inhibition of corrosion by cement-systems, it is highly unlikely that bulk pore water in the cement-rebar system would become anoxic. Therefore, $O_2$ should persist in cement interstitial waters. Once interstitial waters leave the cement environment in water drops, they become hydraulically isolated from the buffering capacity of cement minerals, but are exposed to fresh soil gas that enters the waste zone through the holes in the bottom of the concrete vault. Corrosion of cement rebar has little effect on solution chemistry. However, once water leaves the cement and drips onto carbon steel containers, the cement buffering is removed and steel corrosion can significantly alter solution chemistry.

Table 9. Composition of native Idaho National Laboratory alluvium water that corrodes carbon steel liners after first coming to equilibrium with fresh and mature cement under a soil gas atmosphere. For each type of cement/steel interaction, the range represents the difference between minimum salinity and maximum salinity per Table 2. Water composition corresponds to Point #3 in Figure 3.

| Parameter | pH | Ca-aq (mM) | Mg-aq (mM) | Na-aq (mM) | K-aq (mM) | ΣCO2-aq (mM) | Cl-aq (mM) | SO4-aq (mM) | NO3-aq (mM) | OH- (mM) | Si-aq (mM) | Ionic strength (mM) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Fresh cement | 14.1 | <0.1 | <0.1 | 145–160 | ~950 | ~16 | 0–7.5 | 0.3–7.3 | 0–7.8 | ~800 | ~35 | 940–970 |
| Fresh cement + rebar | 14.1 | <0.1 | <0.1 | 150–170 | ~960 | ~16 | 0–7.5 | 0.3–7.3 | 0–7.8 | ~800 | ~35 | 950–980 |
| Fresh cement+ rebar + carbon steel | 8.4 | <0.1 | <0.1 | 150–170 | ~975 | ~1,100 | 0–7.5 | 0.3–7.3 | 0–7.8 | <0.1 | ~1.5 | ~1,100 |
| Mature cement | 12.4 | ~7 | <0.1 | 1.2–17 | 0-2 | <0.1 | 0–7.5 | 0.3–7.3 | 0–7.8 | 12-15 | <0.1 | 20–50 |
| Mature cement + rebar | 12.4 | ~7 | <0.1 | 1.2–17 | 0-2 | <0.1 | 0–7.5 | 0.3–7.3 | 0–7.8 | 12-15 | <0.1 | 20–50 |
| Mature cement + rebar + carbon steel | 6.5 | ~7 | <0.1 | 1.2–18 | 0-2 | ~30 | 0–7.5 | 0.3–7.3 | 0–7.8 | <0.1 | <0.1 | 20–55 |

When groundwater equilibrated with fresh cement encounters carbon steel liners, fast corrosion would lead to higher ionic strength, reduced pH, and replacement of aqueous OH- anion with aqueous $HCO_3$- anion (originating from gaseous $CO_2$). Some calcite and $SiO_2$ minerals are also likely precipitate. However, it should be noted that these chemical changes are caused by corrosion processes, which are greatly inhibited by high pH. Corrosion will proceed up to 1,000 times more slowly at elevated pH, and the corrosion-induced chemical changes will be concomitantly lower. The only plausible scenario under which corrosion could alter solution chemistry with a fresh cement leachate is if condensation of water vapor in soil gas generated significantly more liquid water in the vaults than groundwater infiltration through the cement.

When groundwater equilibrated with mature cement drips onto carbon steel liners, the changes are similar but of lesser magnitude: solution pH drops significantly, $HCO_3$- anion (from gaseous $CO_2$) replaces the OH- anion, and ionic strength may increase slightly. As with fresh cement, leachate from mature cement has an elevated pH that will inhibit corrosion. Inhibition of corrosion also will reduce the impact of corrosion on solution chemistry. Dilution of cement leachate water with condensed soil vapor would dilute mature cement leachate faster than it would dilute fresh cement leachate (e.g., about 100 times less buffering capacity); therefore, steel corrosion by mature cement leachate is a more likely scenario.

Calculations have also been conducted for groundwater equilibrated with fresh and mature cement dripping onto stainless steel liners. Data for these calculations are not shown, as only carbon steel liners are currently planned for the RH-LLW facility. Data from Adler-Flitton et al. (2004, 2011) indicate that stainless steel corrodes according to a first order rate law, but with a rate coefficient that is approximately 1,000 times lower. At these low rates, the impact of corrosion on solution chemistry is negligible.

## 2.6 Aqueous Geochemical Reactions within Waste Containers (Figure 3, Point #4)

Water entering the waste containers will have a composition that is impacted by native alluvium soils, interaction with cement minerals, rebar, and by interaction with steel waste liners. Given what we know of the system and the corrosion data available; solutions infiltrating into the waste liners are anticipated to have a composition within the range of values specified in Rows 3 and 6 of Table 9. Depending on the content of the waste liners, these solutions will be exposed to one of the following:

- Anion-exchange, cation-exchange, and mixed-bed resins
- Metallic waste
- Miscellaneous waste (e.g., paper products and gloves)
- Mixtures of metals and resins.

Of these waste components, only two will be considered herein: resins and metal parts. Resins should not significantly alter bulk solution chemistry, but will release contaminants into the solution. Corroding metal parts could both alter solution chemistry and release contaminants into the solution. This analysis of the potential solution chemistry within the waste liners will consider three potential interactions between waste forms and the infiltrating solution: (1) release of radionuclides into water from anion-exchange and mixed-bed resins, (2) the impact of corrosion of metal parts on the composition of water that reaches the bottom of the vault, and (3) the possibility that degradation of organic materials in resins and miscellaneous waste might release organic compounds into solution that could form aqueous complexes with radionuclides and enhance transport. With regard to organic materials, miscellaneous waste will be segregated from resins and metallic waste and should not impact geochemical properties within resin and activated metals containers. However, organic resins do degrade radiolytically to produce predominantly gaseous reaction products (Pillay 1986a, Pillay 1986b). These processes will alter the reactivity of the resins, but should not produce aqueous organic moieties that alter sorption within waste containers.

With regards to resins and metallic waste, the large variance in solution chemistry between the fresh cement and the mature cement scenarios complicates these analyses. Ionic strength is over 30 times higher for the fresh cement system than for the mature cement system, and hydrogen-ion concentrations are 100-fold different (e.g., two pH units). These differences have corollary impacts on release of ions from resins and metal corrosion rates. The differing impacts of these two scenarios on radionuclide release require that both fresh cement and mature scenarios be considered.

With respect to anion exchange resins, the processes that occur during radionuclide release and sorption from resins (e.g., Point #4 in Figure 3) only impact contaminant levels and are not expected to significantly alter bulk solution composition. The water compositions in Table 9 (Rows 3 and 6) will be used to calculate the $K_d$ values that control radionuclide release from anion-exchange resins stored within the steel liners. Changes in the oxidation state of the solution are not expected to alter the anion-exchange properties of the resins. The most important solution factor controlling released $K_d$ is anticipated to be the ionic strength of the solution, with higher ionic strength leading to a lower $K_d$. The calculations to estimate $K_d$ calculations for anion release from resins are discussed in Section 3. For activated metals, corrosion both releases contaminants into solution and alters solution chemistry. The water compositions in Table 9 (Rows 3 and 6) will be used to evaluate the impact of metal corrosion on solution chemistry. All corroding metal parts are assumed to be composed of stainless steel. The corrosion rates and associated radionuclide release rates are based on the corrosion data of Adler-Flitton et al. (2004, 2011).

The impact of corrosion on solution composition is estimated with PHREEQc models that predict the composition of the post-corrosion solution that subsequently reacts with the vault floor before moving into the RH-LLW underlayment. To estimate the composition of the post-corrosion solution, each liter of influent water (to the inside of the waste container) from Table 9 is reacted with 1.286 kg of stainless steel, based on the following considerations:

- Total mass of stainless steel, zircaloy, NiCrFe-alloy parts estimated to be sent to the NRF section of the RH-LLW facility is 862,727 kg (Jeff Sondrup, personal communication).
- Along with carbon steel waste containers whose impact on solution chemistry has already been estimated, these parts will be stored in approximately 240,000 $ft^3$ of vault space.
- The NRF portion of the RH-LLW facility is assumed to be emulative of the overall facility. Other sections will contain some aluminum, but the overall percentage of aluminum in the RH-LLW facility is less than 0.5%. Aluminum is assumed to be negligible.
- From this data, there are an estimated 3.6 kg of stainless steel mass per cubic foot of vault space or 128.6 kg stainless steel per cubic meter of vault space.
- Assume a maximum of 10% of total vault space contains water (comparable to estimated moisture content of dry, sandy soil in vault underlayment). This equates to 100 L solution per cubic meter of vault space.

Combining the above bullet points with Adler-Flitton's corrosion data for stainless steel (0.007 grams steel lost per kilogram steel per year, data not shown) equates to less than 2.8 grams steel lost per liter of infiltrating water during the first 500 years, under baseline infiltration scenarios. This steel is lost within corroding waste containers that are water permeable; therefore, it can be reasonably assumed that the air in these containers is able to exchange with the air in the vault and the surrounding soil gas. Thus, as before, this can be modeled as a constant pressure soil-gas system where gas is able to freely exchange. Results from PHREEQc model calculations indicate that corrosion of stainless steel parts within the waste containers should not significantly alter solution composition. This is true regardless of whether or not the infiltrating cement leachate is equilibrated with fresh or mature cement. If the stainless steel parts are sensitized by heat or radiolysis, then corrosion could potentially acidify the exiting water and degrade the cement base more quickly. For as long as cement persists, water exiting the containers and interacting with the floor of the vault will have a chemistry controlled via cement equilibrium.

## 2.7 Water at the Bottom of the Cement Vault (Figure 3, Point #5)

The current design for the RH-LLW vaults calls for four 2-in. diameter holes in the bottom of each vault to facilitate drainage of any water. This means that water will likely be passing over the surface of the cement rather than through the cement matrix itself. This scenario is more similar to the cement revetment described by Fujiwara et al. (1992) than the crack infiltration scenario governing water infiltration into the vault. Thus, cement surfaces at the bottom of the vault are likely to progress beyond the fresh stage more rapidly than surfaces in the cracks that will slowly form in the vault ceiling. Analyses conducted in Section 2.3 of this report highlighted literature studies that suggest that mature cement should persist for over 6,500 pore water exchanges (after fresh cement has been converted to mature cement). Given (1) water minimization activities within the facility during the 50-year performance period will minimize water contact with cement and (2) the 6 to 80 total pore volume flux anticipated to pass through the vault during the 1,000-year performance period of the RH-LLW facility, it is unlikely that cement degradation will progress beyond the mature stage. Therefore, water at the bottom of the vault will likely be interacting with mature cement before moving downward into the vault underlayment.

The RH-LLW facility has a very different hydrologic environment than the revetment investigated by Fujiwara et al. (1992), but it is still possible that the cement surfaces in the bottom of the RH-LLW facility could degrade beyond the mature stage within 1,000 years. Therefore, while mature cement will most likely predominate, degraded cement also will be considered.

## 2.8 Water and Sediment in the Underlayment (Figure 3, Point #6)

As depicted in Figure 1, the RH-LLW vault underlayment is anticipated to consist of sand and gravel at the base of the vault, as well as sand infill between the vault chambers. The mineral composition will consist primarily of aged cement surfaces, sand, and gravel, with sand and gravel providing the dominant reactive surface. Sand is a mixture of quartz, amorphous silica, with a range of soil minerals (e.g., clay minerals and iron oxides) present at low levels, depending on the purity of the sand. These soil minerals will increase the adsorptive capacity of the sand with respect to radionuclide contaminants, but should not significantly alter the major ion composition of the groundwater. Therefore, these minor soil mineral constituents will be assumed absent in all models of the RH-LLW vault underlayment, thereby improving the certainty that $K_d$ estimates will accurately bound the system.

With regards to water, some of the infiltrating water will come in contact with the vault, while other water may pass through backfill before entering the mixing area beneath the vault; where exiting radionuclide contaminants (e.g., vault release water; Point #5 on Figure 3) will enter the RH-LLW vault underlayment. Consequently, the water in the RH-LLW vault underlayment will be a mix of the following:

- Vault release water
- Infiltrating INL alluvium water (from backfill)
- Infiltrating INL alluvium water that has reacted with cement on the vault exterior
- Infiltrating INL alluvium water that has reacted with the engineered cover and infill materials.

The most straightforward way to estimate the solution composition in the RH-LLW vault underlayment is to mix these different waters and then equilibrate the mix with the sedimentary materials in the RH-LLW vault underlayment. Equilibrium calculations are path-independent, meaning the sequence of reactions does not impact the final outcome as long as system boundaries are properly defined. This enables calculation of the solution composition beneath the vault to be conducted in the following four-step process:

1. Calculate the composition of infiltrating INL alluvium water that infiltrates through the engineered cover or sediment backfill before entering the sand/gravel matrix beneath the vault but does not react with cement (Table 2).
2. Calculate composition of infiltrating INL alluvium water in equilibrium with mature cement (e.g., Table 9, Row 4).
3. Calculate the composition of water exiting from the bottom of the vault that has re-equilibrated with mature cement. This is assumed to be the same as infiltrating INL alluvium water in equilibrium with mature cement (e.g., Table 9, Row 4).
4. Mix the two solutions and equilibrate with sand/gravel infill materials.

The chemistry of the resultant solution will vary depending on (1) the sand and gravel minerals assumed to be in equilibrium with the vault underlayment and (2) the mixing ratio of the solutions outlined above. Granite is not a single crystalline mineral, but rather a blend of feldspar, quartz, and minor phases, with the ratio depending on the origin of the granite. For this study, granite was assumed to consist of albite, anorthite, quartz, and K-feldspar. Sand was considered to consist of quartz, calcite, and amorphous $SiO_2$.

The mixing ratio between native INL alluvium water and alluvium water impacted by cement leachate is likely to fall within two bounding scenarios. The first scenario has virtually no lateral interaction between water beneath the cement and water that infiltrates from the sides without interacting with cements. In this scenario, it can be assumed that 95% of the water beneath the vault has equilibrated with cement (Table 9) and 5% has not (Table 2). The second scenario assumes significant lateral exchange, with the water beneath the vault being a 50/50% mix of these two solutions. Once the solutions are mixed, they are equilibrated with a sediment system that is assumed to be 75% sand and 25% gravel. This sand/gravel mix is assumed to have a bulk density of 1,875 kg/m$^3$, porosity of 0.4, and 10% moisture content. Sand is modeled as a mix of 75% quartz, 25% amorphous silica, and trace calcite. Granite is modeled as a mix of 70% quartz, 15% albite, and 15% K-feldspar. All calculations were done in PHREEQc, with water in equilibrium with soil gas (pCO2), fresh cement, and mature cement. Results from these calculations are provided in Table 10.

Table 10. Estimated pH and ionic strength of groundwater in the remote-handled low-level waste alluvium for various scenarios on how cement-impacted water and native alluvium water might mix in the sand/gravel beneath the vault (log pCO2 = -1.25 atm, pO2 = 0.18). For each mix, the ratio corresponds to % cement-water/% native-alluvium-water. Fresh, mature, and degraded refer to stages of cement aging.

| Concrete Type (Cement Impacted Water/Alluvium Water ) | pH | Ionic Strength |
|---|---|---|
| Fresh (95%/5% mix) | Approximately 12.1 | 2,230–2,240 |
| Fresh (50%/50% mix) | Approximately 12.0 | 1,120–1,130 |
| Mature (95%/5% mix) | Approximately 11.8 | 60 to 80 |
| Mature (50%/50% mix) | Approximately 6.9 | 30 to 60 |
| Degraded (95%/5% mix) | Approximately 11.2 | 40 to 55 |
| Degraded (50%/50% mix) | Approximately 6.7 | 30 to 45 |

These data suggest that solution chemistry (and $K_d$) will strongly depend on mixing between native alluvium water and water that has been in contact with cement surfaces. The 95% cement-water, 5% alluvium-water is the most likely scenario for the sand and gravel layer beneath the vault. However, the 50/50% mix scenario could occur if the engineered cover is intact limiting infiltration through the vault and significant lateral inflow occurs as a result of higher than normal precipitation or overland flooding.

## 2.9 Water and Sediment in the Alluvium Beneath the Vault Underlayment (Figure 3, Point #7)

The RH-LLW vault and sand/gravel underlayment is anticipated to rest within an approximately 55-ft thick layer of native INL alluvium. This material will have a different hydraulic conductivity and different surface chemistry than the sand/gravel underlayment. However, the solution chemistry will be impacted by the same mixing factors as those impacting the vault underlayment. Therefore, mixing between cement-leachate water and native alluvium water will control pH, ionic strength, and contaminant sorption. $K_d$ values for radionuclide sorption to the sediment will be estimated for the same bounding water compositions as for the RH-LLW vault underlayment (Table 10).

Sediment in the RH-LLW alluvium is anticipated to fall within the compositional range of surficial sediment located elsewhere in INL. In general, INL surficial sediment is a calcareous silty-clay under the unified soil classification system. The grain size distribution is variable. For fine-grained sediment, most samples have 35 to 75% (by mass) within the silt size fraction. Depending on sample and extraction method used, surficial sediment contains 0.3 to 6 mg iron-oxide iron per gram of sediment. Prior x-ray diffraction analyses (Fox et al. 2004, Plummer et al. 2004) have indicated that samples of INL surficial sediment are 50 to 75% quartz, 10 to 25% plagioclase and K-feldspar, 10 to 20% clay minerals, less than 5% olivine and pyroxene, less than 5% calcite, and less than 5% iron oxides. The fine grain size fraction (less than 75 μm) is approximately 40 to 55% quartz, 30 to 45% clay minerals, 5 to 10% plagioclase and K-feldspar, 5 to 10% calcite, and less than 5% iron oxides with trace amounts of gypsum and other minerals. The clay minerals are predominantly mixed illite-smectite (50 to 75%), with kaolinite, illite, and Ca-rich smectite comprising the remaining fraction. With regards to radionuclide sorption, Leecaster (2002) report that $K_d$ values for uranium and neptunium are most tightly correlated to the following:

- *For neptunium*: Exchangeable calcium, extractable iron oxides, kaolinite fraction of clay, and sum of exchangeable cations (e.g., cation exchange capacity [CEC]). Exchangeable Ca explained approximately 65% of the variability in measured neptunium $K_d$ values.
- *For uranium*: Exchangeable calcium, exchangeable magnesium, extractable iron oxides, extractable manganese oxides, illite fraction of sediment, smectite fraction of clay, and sum of exchangeable cations (e.g., CEC). CEC explained approximately 50% of the variability in measured uranium $K_d$ values.

Based on these results, sorption for different radionuclides can be expected to correlate with different combinations of sediment parameters. No single sediment parameter is expected to be predictive of $K_d$ values. However, many of these parameters are directly or indirectly related to CEC, which is a measure of the reactivity of clay mineral surfaces. Prior research suggests that radionuclide sorption to INL sediment is controlled by reactions between aqueous radionuclides, clay minerals, and carbonate minerals, and likely is controlled by the following four types of processes (e.g., Leecaster and Hull 2003, Mincher et al. 2003, Mincher et al. 2004, Hull et al. 2004, Hull and Schafer 2008, Hull and Pace 2000):

- Radionuclide ion-exchange with clay mineral surfaces
- Radionuclide surface complexation with SiOH, AlOH, and FeOH reactive sites on clay mineral and iron oxide surfaces
- Radionuclide partitioning into carbonate minerals via precipitation and co-precipitation reactions
- Radionuclide precipitation as oxyhydroxide minerals.

Organic moieties also may contribute to sorption. However, INL sediment has low organic content and organic materials are thought to be of minor importance. Within INL sediment, clay minerals are the dominant reactive surface and both ion-exchange and surface complexation reactions and sorption should correlate positively with the reactive surface area of clay minerals. Precipitation reactions are catalyzed

by fine-grained mineral surfaces that can reduce the activation energy of surface precipitation reactions. Therefore, partitioning into carbonate and oxide phases should also correlate somewhat with the abundance of clay mineral surfaces, though any correlation between CEC and mineral precipitation reactions will be less than for ion-exchange and surface complexation reactions. Based on this reasoning, radionuclide adsorption in INL interbed and alluvium sediment should generally correlate with the concentration of reactive sites on clay minerals. One measure of this is CEC. Direct correlation between metal and radionuclide partitioning and CEC of clay-dominated soils has been observed at other locations (Kamel 2010, Usman 2008, Holm et al. 2003, Ohnuki 1994), and CEC has been observed to correlate positively with Np and U sorption to INL sediment (Plummer et al. 2004). Thus, while $K_d$ cannot be predicted from CEC, it is reasonable to extrapolate the applicability of $K_d$ values measured for sediment at various INL locations and other sites with comparable mineralogy to interbed and alluvium sediment at the Advanced Test Reactor (ATR) Complex based on CEC.

Cation exchange capacity (CEC) values within INL surficial sediment (Figure 7) range from approximately 3 to 40 meq per 100 grams, with most sediment having a CEC of less than 15 meq per 100 g. The sitewide distribution is skewed toward lower CEC values. In the region near the ATR Complex, CEC ranges from approximately 3 to 30 meq per 100 g, with most sediment having a CEC that ranges from 5 to 15 meq per 100 g. Recently gathered geotechnical data (American Geotechnics 2011) indicates that the average CEC in the proposed location is 9.3 meg/100g, increasing with depth. For shallow samples (depth less than 33 ft), the mean is 6.4 meq/100g. For deeper depths, the mean is 11.7 meq/100g. The distribution shown in Figure 7 does not include the recent geotechnical data and is more uniformly distributed than the sitewide values. However, the most probable range of CEC values correlates well with sitewide data and with the recent geotechnical data. Therefore, $K_d$ values for alluvium sediment within the ATR Complex are likely to be consistent with values measured elsewhere on the site, as long as CEC and solution composition also are comparable.

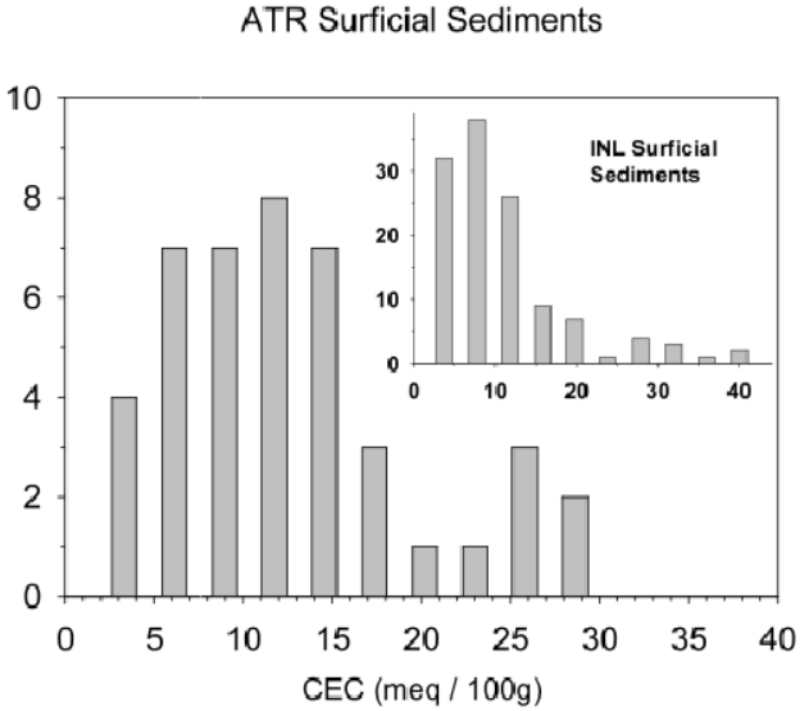


Figure 7. Histogram of measured cation exchange capacity values for surficial sediment at the Advanced Test Reactor Complex (n = 43) and Idaho National Laboratory sitewide (inset, n = 122).

## 2.10 Water and Sediment in the Sedimentary Interbeds

As depicted in Figure 1, sediment interbeds are layers of INL sediment sandwiched between layers of basalt in the deep vadose zone that separate the alluvium from the aquifer. The groundwater and mineral composition of this region is estimated from historical data collected from groundwater monitoring wells and sediment cores. Alteration of alluvium during construction of the vault and ongoing site operations are assumed to not impact the composition of groundwater in sediment interbeds.

The ion chemistry of groundwater in INL interbed sediment is presented in Table 11. These data indicate that the ion composition is variable, with non-normal distributions. Oxidation potentials and pH values are rarely reported, and pH values often must be calculated from measurements of alkalinity and aqueous $CO_2$. In contrast to alluvium water, interbed groundwater has a lower ionic strength, with calcium and bicarbonate being the predominant ions. The Ca:Mg ratio is much higher, and sodium and sulfate concentrations are much lower. This is consistent with a process whereby highly soluble sodium and sulfate ions are washed into the aquifer faster than calcium, magnesium, and bicarbonate ions, whose solubility is controlled by carbonate mineral precipitation. In areas close to the Big Lost River, interbed sediments can be affected during wet years. However, that infiltration also occurs through the alluvial sediments. In general, the chemical processes dominant in interbed groundwater will be similar to those for alluvium groundwater; but with lesser impact from soluble salts.

Table 11. Composition of interbed water at the Advanced Test Reactor Complex, with variance statistics as data allow. Because of inconsistent data collection, total cation and anion data are minimum values. Data was gathered from wells at the Advanced Test Reactor Complex that are outside the facility fence line (Well Numbers USGS-62, USGS-66, USGS-71, and USGS-78).

| Parameter | pH | Ca++ (mM) | Mg++ (mM) | Na+ (mM) | K+ (mM) | HCO3- (mM) | Cl- (mM) | SO4-- (mM) | NO3- (mM) | Cations (meq/L) | Anions (meq/L) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Minimum | — | 0.0 | 0.0 | 0.0 | 0.0 | — | 0.0 | 0.1 | 0.1 | 0.0 | 0.3 |
| Maximum | — | 3.7 | 1.3 | 0.8 | 0.2 | — | 0.6 | 2.3 | 1.5 | 10.7 | 7.5 |
| Median | 7.5 | 2.8 | 0.9 | 0.3 | 0.0 | 1.1 | 0.1 | 0.2 | 0.5 | 0.3 | 0.5 |
| n | 2 | 8 | 8 | 25 | 8 | 2 | 23 | 21 | 4 | 25 | 21 |
| % deviation from median* | — | 50% | 53% | 77% | 163% | — | 128% | 345% | 124% | 1,274% | 358% |
| Skewness | — | -1.1 | -1.0 | 1.2 | 2.3 | — | 2.2 | 2.2 | 1.0 | 1.4 | 2.4 |
| Kurtosis | — | -0.4 | -0.42 | 1.0 | 5.9 | — | 3.6 | 3.5 | -0.4 | 0.1 | 4.8 |

* Interbed water samples include those likely influenced by anthropogenic water sources, Big Lost River water, and natural precipitation, contributing to the overall variability.

Sitewide, the composition of INL interbed sediment ranges from silty-clays to clay-bearing sands under the unified soil classification system. Reactive phases are dominantly calcite and a heterogeneous mixture of illite, smectite, kaolinite, and mixed layer clays, with no clear trends in mineralogy, grain size distribution, or cation exchange capacity (Lewis et al. 1992, Bartholomay et al. 1989, Bartholomay and Knobel 1989, Bartholomay 1990, Reed and Bartholomay 1994).

Cation exchange capacity (CEC) values for interbed sediment near the ATR Complex and sitewide across INL are presented in Figure 8. Little CEC data exist for the ATR Complex, with available data indicating that CEC ranges from 2 to 15 meq/100 g. These values are comparable to sitewide values that typically range from 2 to 25 meq/100 g, but the average value for ATR sediment is lower than the sitewide distribution, which has outliers as high as 45 meq/100 g. Based on limited data, the distribution of measured CEC values in ATR interbed sediment is flatter than the sitewide CEC distribution, which is skewed toward lower values. These data suggest that, while the median CEC of interbed sediment near the ATR Complex may be somewhat lower than the median value sitewide, the sediment composition is comparable. Additionally, the CEC distribution of interbed and alluvium sediment also is consistent with each other both sitewide and within the ATR Complex. Consequently, $K_d$ values should be comparable

between these two different sediment layers as long as solution composition also is comparable. With regards to interpolation of $K_d$ values from experiments conducted on sediment from places other than INL, values can be expected to be reasonably comparable if the sediment used is a calcareous silty-clay, with CEC values that range from 5 to 15 meq per 100 g.

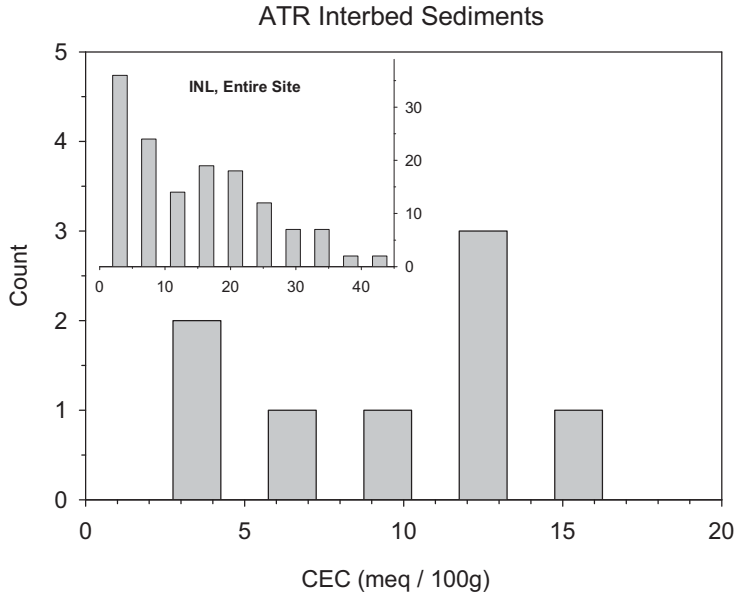


Figure 8. Histogram of measured cation exchange capacity values for interbed sediment at the Advanced Test Reactor Complex (n = 8) and sitewide (inset, n = 138). Advanced Test Reactor data are from wells PW-10, PW-11, TRA-05, TRA-06, and TRA-07; ranging from 140 to 220 fbs per Table 3-7 of Lewis et al. (1992).

# 3. DETERMINATION OF DISTRIBUTION COEFFICIENTS

The transport model used in the performance assessment for the RH-LLW disposal facility is based on a $K_d$ formulation requiring $K_d$s to be assigned to each media contacted by radionuclides. This section describes how these $K_d$ values are determined on the basis of the solution and solid-phase parameters discussed in Section 2.

## 3.1 Distribution Coefficient Values for Release of Radionuclides from Anion-Exchange Resins in the Vault

This subsection describes the derivation of the parameters that describe resin properties and subsequently describes how $K_d$ is calculated from the physical properties of the resins and the composition of groundwater that has infiltrated into the vault and waste containers. The conceptual model assumes that (1) resins release adsorbed radionuclides according to an ion-exchange process, (2) the chemical properties of the resins change as the resins degrade radiolytically, and (3) the chemistry of the exchange reaction(s) is subsequently impacted by radionuclide degradation.

### 3.1.1 Chemical and Physical Properties of Fresh Resins

The waste forms to be stored in the vault include anion-exchange, cation-exchange, and mixed-bed resins from the ATR Complex and NRF facilities. The screening process used to down-select radionuclides for detailed assessment screened out all resin-associated nuclides, except technetium and iodine. Thus, only anion-exchange and mixed-bed resins will be considered herein. These resins are hygroscopic, macroporous beads that retain water within their pores even after they have been air-dried at

room temperature. The pores within the beads give the beads greater structural integrity, but do not contribute significantly to the chemical reactivity.

The anion exchange resins used at the ATR and NRF complexes come from a number of processes whose purpose is to remove a broad spectrum of radionuclides from cooling water used in the INL's Advance Test Reactor Complex and Naval Reactor Facilities (SPC-51590). The technical specifications (SPC-51590 and ECAR-526) set performance requirements for resins at the ATR Complex based on the following parameters: (1) operation at elevated temperature, pressure, and radiologic dose, (2) macroporous structure with a defined chemical composition, (3) defined percentage of whole beads and particle size, (4) defined friability (resistance to crushing/fracturing), (5) defined ability to retain moisture, (6) defined overall exchange capacity, and (7) defined percentage of the total exchange capacity (e.g., anion or cation exchange capacity) as a given ionic compound.

The engineering specifications for the resins do not require that they have a special affinity for a target radionuclide, and chemical data to describe the relative affinity of the resins for different anions is not available. Scaling factors are used to estimate radiologic dose from technetium and iodine (ECAR-130), but these factors are based on gamma radiation and not resin chemistry. The dose from technetium and iodine on anion-exchange resins is scaled from the measured dose from Cs-137 and Co-60 cations on the basis of imprecise empirical data and provides a reasonable basis for estimating the total dose accumulated by the resins. However, this approach does not provide chemical information that can be reliably used to estimate the chemical affinity of fresh beads for iodine and technetium anions in competition with other solution anions. Structurally, the anion resins are "styrene-divinylbenzene copolymer functionalized with trimethylamine to form a quaternary." This is a relatively standard synthetic organic ion-exchange resin used in the nuclear industry. Such resins are stable at elevated temperature and pressure, insoluble in organic solvents, and widely considered to be inert in soil environments. However, according to material safety data sheets for ATR resins and DOWEX beads with physical properties comparable to the resins used at the ATR Complex, such resins can react with strong oxidizing agents (such as concentrated nitric acid) and experience some surface photodegradation in sunlight. Thus, while these resins should be relatively inert in a typical soil environment, they may degrade in a radiologic environment.

Table 12. Vendor data for cation and anion-exchange resins used at the Advanced Test Reactor Complex, derived parameters for estimating a distribution coefficient for radionuclide release, and results from comparable anion resins disposed of at the Subsurface Disposal Area.

| Vendor Data (Resintech Inc.) | | | | | | | Calculated Parameters | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Reference | CAS# | Cation or Anion | Volume Basis Exchange Capacity (meq/cc) | Void Space (cc/cc) | Percent of Resin that is Water | Shipping Weight (lb/cf) | Grain Density (g/cc resin) | Bulk Density (g/cc total) | Mass Basis Exchange Capacity, Moist Resin (meq/g) | Mass Basis Exchange Capacity, Dry Resin (meq/g) |
| INL MSDS, 030308 | 69011-20-7 | Cation | 1.7 | 0.35 | 45–55 | 50 | 0.80 | 0.52 | 3.2 | 4.5–5.0 |
| INL MSDS, 031447 | 69011-18-3 | Anion | 1.1 | 0.35 | 52–60 | 43 | 0.69 | 0.43 | 2.6 | 3.2–4.1 |
| INL MSDS, 031449 | 69011-20-7 (cation, 42%) | Mixed bed | 2.0 | 0.35 | 50 | 44 | 0.70 | 0.52 | 3.8 | 5.6 (cation) |
| | 69011-18-3 (anion, 58%) | | 1.5 | | | | | | 2.8 | 4.2 (anion) |
| Hull 2004 | none | Anion | 0.9 | 0.31 | — | — | 0.68 | 0.47 | 2.8 | — |

General chemical and physical properties of the ATR resins, and for comparable resins buried in RWMC (Hull 2004), are given in Table 12. Both vendor data and derived values are provided. The calculated parameters in Table 12 are derived from vendor data using Equations 2 through 5 and are provided to facilitate intercomparison with other resin types.

Grain density = density of dry resins at room temperature, calculated by converting the shipping weight to units of grams per cubic centimeter (2)

Bulk density = grain density * (1 – void space), term refers to the mass of resins per unit volume in a packed column (3)

Mass-basis exchange capacity of moist resin = volume-based exchange capacity/bulk density, term refers to equivalents per gram when moist (4)

Mass-basis exchange capacity of dry resin = volume-based exchange capacity/bulk density –void space*[1-fraction of resin that is water]), term refers to equivalents per gram when all water has been driven off. (5)

### 3.1.2 Radiolytic Degradation of Anion-Exchange Resins

Pillay (1986a, 1986b) provides a review of the stability of ion-exchange resins in radiologic environments. Ionizing radiation doses on the order of $10^5$ to $10^6$ Gray (Gy) ($10^7$ to $10^8$ rad) are known to significantly alter the properties of synthetic organic ion-exchange resins. The effects are dependent on several factors, including (1) chemical composition of the resin, (2) ionic form of the exchanging ions, (3) moisture content, (4) swelling characteristics, the (5) degree of cross-linkage in the macromolecular structure, and (6) the characteristics of the radiation source. These factors impact the rate and mechanism of degradation and the chemical impact of this degradation. Different commercial resins have different chemical structures and will react differently. However, some general trends are consistent for all types of synthetic organic resins. Radiolytic degradation of amine-functionalized resins results in (1) evolution of volatile free amines, (2) release of corrosive or reactive gases such as $H_2$ and CO, (3) decrease in swelling capacity, (4) loss of exchange capacity, and (5) general degradation of the resin matrix. As noted previously, the degradation products will likely enhance the rate of steel corrosion in the liners. The resins themselves also will lose chemical functionality, including loss of total exchange capacity. The design specifications for ATR resins (SPC-51590) require that the resin retain full functionality at doses of up to $1.0 \times 10^6$ rad ($10^4$ Gy). Therefore, we will assume that all resins will have received this dose at the point they are transmitted to the facility. There are two possible exposure scenarios once the technetium and iodine-bearing resins have been interred within the RH-LLW facility:

1. *Resins exposed to radionuclides in resin containers only.* This scenario occurs if two resin containers are stored together in the same vault. . Radiological records from Integrated Waste Tracking System reports for these resins indicate that the vast majority has a contact dose of less than 3,000 mrem/hour when the containers are transported for disposal, with only a rare outlier exceeding that value. Most of the contact dose originates with Co-60 (half-life of 5.27 years, decay constant of 0.1315 /yr). If it is assumed that two containers are placed in each chamber and most of the dose received by the moist resins comes from beta and gamma radiation (e.g., 1 rem = 1 rad), then are two ways to estimate total absorbed dose over time.
    a. The contact dose rate of 3,000 mrem/hourr equates to a probable maximum dose rate of 52,560 rad/year (6,000 mrad/hour). At this rate, it would require 172 years to reach a dose of $10^7$ rad, which is the point at which the effects of ionizing radiation are known to alter the chemical properties of the resins (*note*: the absorbed dose at the time of disposal is $10^6$ rads).
    b. The calculation based on the probable maximum dose rate does not consider shielding from the steel containers, or radioactive decay that will reduce the dose rate over time.

c. Most of the gamma exposure rate is from Co-60 (half-life of 5.27 years). The time to reach $10^7$ rads accounting for radioactive decay is given by the following equation:

$$t = \frac{-\ln\left(1 - \frac{\lambda D}{\dot{D}}\right)}{\lambda}$$

where $\lambda$ = the radioactive decay constant (1/yr), D = $10^7$ rads, and $\dot{D}$ = the initial dose rate (52,560 rad/yr). Using these values in the above equation results in a infinite time to reach $10^7$ rads. The total dose received would be ~$4 \times 10^5$ rads. Therefore, resins exposed only to radionuclides contained in the resins would not be expected to exceed a total absorbed dose of 1.5 x $10^6$ rads. This is less than the total dose of $10^7$ rads, which is the minimum dose known to stimulate radiolytic decay, but this lower dose could still catalyze chemical degradation via reaction paths that Pillay (1986a, 1986b) did not consider.

2. *Resins exposed to radionuclides in resins and activated metals.* This scenario occurs if one resin container and one activated metal container are stored together in the same vault. The maximum contact exposure rate for activated metals is estimated to be 30,000 R/hour (Carlson et al. 2006), where most of the exposure rate is from gamma photons emitted from Co-60. Based on calculations using the Microshield code and assuming two 0.342 cm steel liner walls, an attenuation factor of 0.813 was calculated. Assuming 1R ~ 1 rad, the contact dose rate of 30,000 R/hour equates to an initial maximum dose rate of $2.13 \times 10^8$ rad/year. At this rate and allowing for radioactive decay, it would require approximately 2 weeks to reach a dose of $10^7$ rad.

Radiolytic degradation will (1) alter the chemical functionality of organic moieties that may exhibit a higher chemical affinity for the target radionuclides than for other ionic species, and (2) decrease the total ion-exchange capacity of the resin. With regards to chemical affinity, this analysis assumes that the resins do not have a special affinity for a target radionuclide. This is consistent with the absence of chemical affinities specified in the engineering design documents (SPC-51590) and the broad array of processes that generate waste resins. It also accommodates the impact of radiolytic degradation on resin chemistry. This assumption of no affinity implies that the $K_d$ of the resins is solely based on the anion-exchange capacity of the resin and the total anion charge concentration in solution. This is conservative (e.g., underestimates $K_d$), because higher $K_d$ values would be observed if the resins exhibited selectivity for iodine and technetium over other solution anions.

With regards to loss of ion-exchange capacity as a function of absorbed dose, Pillay (1986a, 1986b) provides a thorough summary of prior experiments investigating the impact of radiation on resin degradation, including data on loss of ion-exchange capacity. These data demonstrate a range in the rate-of-loss of ion-exchange capacity in response to radiolytic degradation, with the deleterious impacts of ionizing radiation on ion-exchange capacity beginning at an absorbed dose of $10^6$ Rad. This threshold is approximately 10 times lower than the $10^7$ Rad threshold discussed above. However, Pillay (1986a) notes that the degradation rate consistently decreases with increasing extent of polymeric cross-linking. The engineering specifications (SPC-51590) do not require a degree of cross-linking, but they do require that the resins maintain chemical functionality at an elevated radiologic dose. Thus, it is reasonable to assume that more highly cross-linked resins would be used in nuclear operations and that current resins are more stable than the 25-year old resins assessed in the studies reviewed by Pillay (1986a, 1986b). Such resins would have improved performance and provided for safer operations because a reduced degradation rate also prevents the formation of $H_2$ gas. Given this, it is likely that the resins used in the ATR Complex and NRF will not degrade more rapidly than the "typical" wet or moist anion-exchange resins with a predominantly $OH^-$ anionic form used over 25 years ago, as reported by Pillay (1986b).

Data from Pillay (1986a, 1986b) are presented in Figure 9. These data indicate an exponential loss of exchange capacity with increasing dose, suggesting a first-order reaction mechanism where the loss rate is dependent on the initial exchange capacity. Pillay (1986b) compared data from multiple experiments and

normalized all data to the initial exchange capacity (e.g., reported as proportion of exchange capacity lost) in order to assess trends across as many datasets as possible. This dataset suggests that 90% of the total exchange capacity will be lost by the time the beads receive an integrated dose of $1.0 \times 10^9$ rad and 95% may be lost by the time the beads receive a dose of $2.0 \times 10^9$ rad. Applying these degradation data to the two exposure scenarios previously outlined yield three potential impacts on resin chemistry:

- *Resins exposed to radionuclides in resins and activated metals.* Resins are exposed to a probable maximum dose rate of $2.63 \times 10^8$ rad/year. Resins could lose chemical functionality in less than 1 month and would have a $K_d$ of 0 mL/g.
- *Resins exposed to radionuclides in resins only and only decay via radiolytic processes.* Resins are exposed to a probable maximum dose rate of 52,560 rad/year (6,000 mrad/hour), but shielding and radioactive decay prevent resins from receiving a total absorbed dose in excess of $10^7$ rad. Resins do not exceed the minimum dose for radiolytic degradation, retain chemical functionality well beyond the institutional control period, and will have a non-zero $K_d$.
- *Resins exposed to radionuclides in resins only and decay via a combination of radiolytic and biogeochemical processes.* The dose scenario is the same as for resins being exposed to resins only, but radiolysis stimulates a number of other chemical and microbiological processes that slowly degrade the resins at an unknown rate. The net rate of degradation can be assumed to be less than that for extended radiolysis at the maximum dose rate (52,560 rad/year); therefore, continued exposure at this level provides a conservative upper bound for resin degradation.

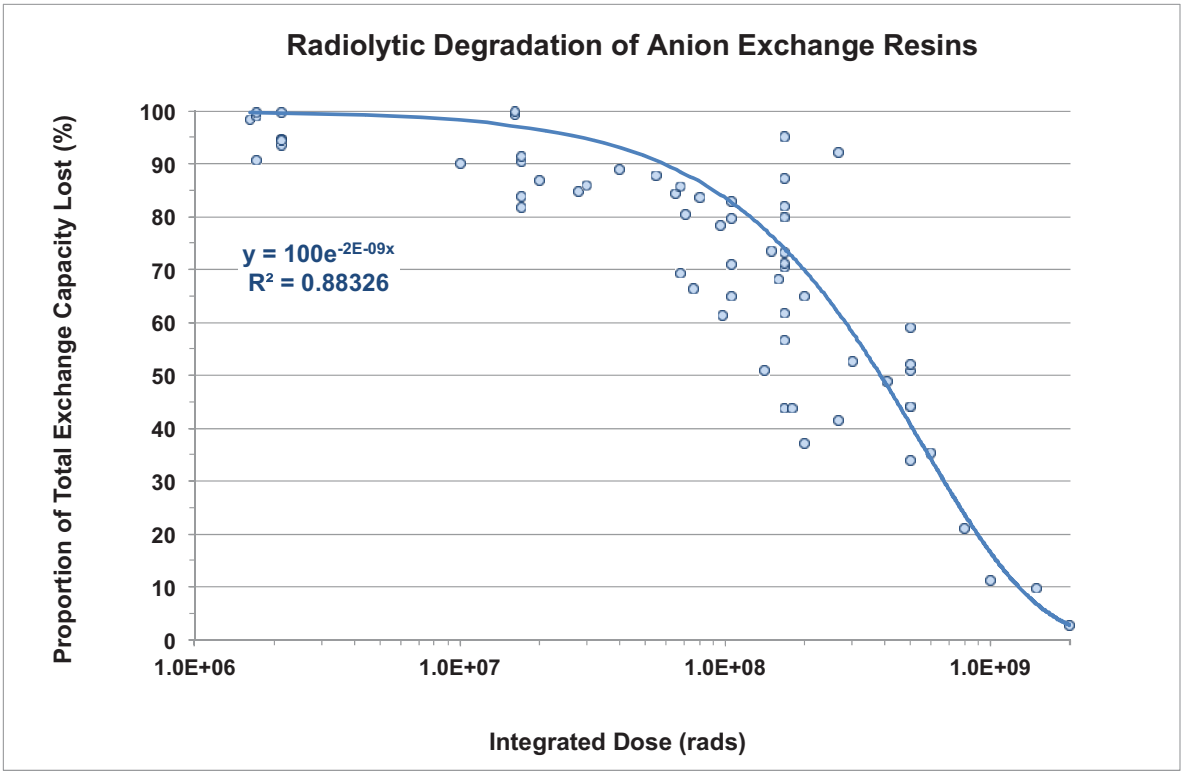


Figure 9. Loss of total anion-exchange capacity as a function of integrated dose for wet or moist anion-exchange resins with a predominantly OH- anionic form, as reported by Pillay (1986b). All resins were styrene divinylbenzene copolymers with varying functionalization and extent of cross-linkage.

Resins that are exposed to contact dose rates from activated metals will not retain technetium and iodine ($K_d$ 0 mL/g). Dose rates for resins that are only exposed to radionuclides in other resins will be much lower; therefore, resins will retain chemical functionality and have a non-zero $K_d$. If it is assumed

that resins do not degrade over time, then the ion-exchange capacity of the resins (resin-IEC) will not change over time. If it is assumed that the resins do degrade, then resin-IEC will be reduced over time. With degrading resins, the resin-IEC used to calculate $K_d$ can be estimated by calculating either the average or median resin-IEC over a time period that is relevant to the transport properties of iodine and technetium. Three time periods should be considered when deciding what is representative: (1) the time period that it takes for the steel liners to corrode, (2) the time period during which all iodine and technetium could be released from resins, and (3) the time period when the exchange capacity of the resins fully decay:

1. *Corrosion of 10 gauge steel liners.* Initial corrosion calculations suggest that 25% of ATR resin liners could fail within 1,000 years, 50% of liners could fail within 1,500 years, 75% could fail within 2,000 years, and 100% will fail within 5,000 years (personal communication, Jeff Sondrup, Idaho National Laboratory, December 2010).
2. *Loss of technetium and iodine from resins*. Initial calculations under aggressive leaching scenarios (e.g., leachate from "fresh" cement) that assume a non-degrading anion-exchange resin (e.g., constant anion-exchange capacity) indicate that all technetium and iodine associated with resins should exit the waste containers and cement vault within 10,000 years (personal communication, Jeff Sondrup, Idaho National Laboratory, December 2010).
3. *Complete radiolytic degradation of ion-exchange resins*. If resins decay via a combination of geochemical and microbiological mechanisms at a rate slower than simple radiolytic decay at the initial dose rate, then a maximum likely decay rate can be estimated by applying a dose rate of 52,560 rads/year to the equation derived in Figure 9. In this case, the ion-exchange capacity of the resins would be exhausted sometime after 50,000 years of internment.

Resins will no longer impact transport of technetium and iodine after 10,000 years; therefore, the 50,000-year timeframe for loss of resin-EC is irrelevant. Resin decay only needs to be considered for the first 10,000 years. This analysis will provide estimates of average and median ion-exchange capacities for five scenarios:

1. *Resins maintain their initial exchange capacity for the first 10,000 years of internment*. Resins retain their initial ion-exchange capacity of 1.1 meq/cc (volumetric basis, minimum of Table 12).
2. Resins degrade at a rate less than radiolytic decay at a dose rate of 52,560 rads/year, for a period of 0 to 1,500 years. The minimum time-averaged, ion-exchange capacity is estimated to be 1.02 meq/cc and the median value is 1.02 meq/cc.
3. Resins degrade at a rate less than radiolytic decay at a dose rate of 52,560 rads/year, for a period of 1,500 to 5,000 years. The minimum time-averaged, ion-exchange capacity is estimated to be 0.79 meq/cc and the median value is 0.78 meq/cc.
4. Resins degrade at a rate less than radiolytic decay at a dose rate of 52,560 rads/year for a period of 5,000 to 10,000 years. The minimum time-averaged, ion-exchange capacity is estimated to be 0.51 meq/cc and the median value is 0.50 meq/cc.
5. *Resins are co-located with activated metals in the same vault.* All ion-exchange capacity is lost within 1 month, and ion-exchange capacity is 0 meq/cc (implying a $K_d$ of 0 mL/g).

### 3.1.3 Calculation of $K_d$ from Resin Properties Impacted by Degradation

These calculations assume that the anion-exchange resins will release technetium and iodine into solution via an anion-exchange mechanism where the chemical functionality of the resins is slowly lost as the resins degrade radiolytically. As previously discussed, the chemical impact of radiolytic degradation of anion-exchange resins on radionuclide release is estimated based on the following assumptions.

1. It is assumed that the anion-exchange resins in the vault have no selectivity for radionuclide anions, and all anions will interact equally with the beads. This means that $K_d$ is a simple ratio between the total anion charge in solution and the total anion-exchange capacity of the resins.
2. Three assumptions governing resin degradation are considered: (1) resins do not degrade, (2) resins degrade at a rate less than that of radiolytic decay, and (3) resins are exposed to activated metals and degrade completely within a period of 1 month.
3. For cases where the resins degrade, the estimated median ion-exchange capacity over three different timeframes is adopted instead of the initial ion-exchange capacity (estimated minimum of 1.1 meq/cc; Table 12). The median exchange capacity is adopted, because it is lower than the average and will yield a more conservative $K_d$ estimate.

A $K_d$ value that is applicable to a given scenario can be estimated from the median ion-exchange capacity of the beads and the anion charge concentration of the infiltrating water that has penetrated into the liners (Table 9) using Equation 6:

$$K_d \text{ (mL/g)} = ((EC_{vol}/\Sigma \text{ anions}) - 1) * (\text{void space/bulk density}) \quad (6)$$

Where:

$EC_{vol}$ = exchange capacity of the column, volumetric basis in units of meq/cc

$\Sigma$ anions = anion charge concentration in pore water in units of meq/cc

Void space = pore space of the resin bed in units of cc/cc

Bulk density = bulk density of resin bed and surrounding materials in units of g/cc

Note: cc = cubic centimeter = mL.

This equation is derived by assuming that the retention factor for transport of any anion in an anion-exchange column is equal to the ratio of anion-exchange capacity to total aqueous anion concentration and then calculating $K_d$ from the retention factor. The assumption that the retention factor is the ratio of total adsorbed charge to total aqueous charge treats all anions equally, regardless of their inherent chemical differences. One notable effect of this approach is that changes in the aqueous concentration of technetium or iodine do not alter $K_d$ because such a change would have to be offset by adsorption of a different anion to maintain charge balance; and the total charge concentration in solution would remain the same for any aqueous system where water mass is constant and/or soluble minerals do not precipitate or dissolve.

This approach is technically inaccurate because each anion has a specific chemistry and will competitively adsorb to the resin with respect to other anions. However, the chemistry of degrading resin and of their interaction with radionuclides of interest and major aqueous anions is not known for the time-changing specific environment of the RH-LLW disposal facility. Thus, a comprehensive anion-exchange model that accounts for chemical affinities cannot be reliably used.

Assuming that iodine and technetium exhibit no chemical affinity for the resin is conservative so long as the dominant ions in solution (OH-, $CO_3^{2-}$, Cl-, $SO_4^{2-}$) do not have a higher affinity for the resin than do the radionuclides. Given that the technical specifications for the resins (SPC-51590) require the resins to use OH-, $CO_3^{2-}$, Cl- and $SO_4^{2-}$ as counter ions in a resin that is used to remove aqueous technetium and iodine from reactor solutions, it is likely that these radionuclides adsorb more strongly to the resin than do the counter anions. Finally, this approach inherently assumes that ions exchange on a one-for-one charge basis, as would occur if a -1-charged solution ion exchanged with a -1-charged adsorbed ion. However, different solution and radionuclide species have different formal charges that will impact the strength of sorption. This issue would become problematic if -2-charged anions, such as $SO_4^{2-}$ or $CO_3^{2-}$ were to comprise a large portion of the solution and enhance desorption of I-, $IO_3$- or $TcO_4$-. Model results

presented in Table 9 indicate that -2-charged anions will only exceed 2% of total solution anions in cases where mature cement degradation controls solution chemistry and high $SO_4^{2-}$ levels are present. Even then, -2-charged anions would only constitute approximately 25% of total solution anions. The impact of -2 anions on $K_d$ is likely to be lower than the uncertainty inherent in these calculations and not likely to reduce actual $K_d$ below that predicted based on the bounding conditions used in this study. Consequently, this approach should provide accurate bounding calculations as long as formation of mineral or organic coatings on the beads does not degrade the anion exchange capacity or generate anionic species whose affinity for the resins is significantly higher than that of iodine and technetium.

With regards to coatings, evidence from the literature suggests that non-selective resins may react with groundwater contaminants to form nonreactive coatings and deactivate faster than highly selective resins. For example, Gu et al. (2000) observed that the Purolite resins they employed in a Tc-99 field study at Oak Ridge National Laboratory accumulated three times more $SO_4^{2-}$ than resins that were highly selective for Tc-99, even though they processed about three times less groundwater. This type of behavior may facilitate the formation of $CO_3^{2-}$ and $SO_4^{2-}$ minerals on the surface of the beads, thereby altering sorption properties in a way that may impact $K_d$. Mineral precipitates passivate reactive surfaces, thereby making them less able to remove contaminants from solution. This same process also will reduce the extent to which passivated surfaces release contaminants into solution. Consequently, the formation of mineral precipitates should act to increase a release $K_d$. Lower $K_d$ values are more conservative; therefore, this analysis assumes that reactive coatings will not impact the release $K_d$. With regards to anionic species that could reduce sorption of iodine and technetium to resins, the major source of such species would be from radiolytic degradation of the resins. This process generates methylamines and reactive gasses (Pillay 1986a), and there are no data to suggest that formation of these products would impact radionuclide sorption to resins in a way that has not been accounted for in prior analyses.

Based on these arguments, a conservative bounding estimate for the resin release $K_d$ can be calculated from the ion-exchange capacity of the beads and the total anion-charge concentration of the infiltrating water. For each time period described in Section 3.1.2, the anion composition of the solution will be variable and dependent on the extent of aging cement leaching and steel corrosion in the waste containers. $K_d$ values will be estimated for each combination of time period, cement leaching, and steel corrosion. $K_d$ values for the initial condition (no degradation of anion-exchange resins) also will be provided for comparative purposes. Solution compositions expected to be reflective of the maximum possible extent of steel corrosion are presented in Table 9 (Rows 3 and 6) for fresh and mature cement. These ranges are used to estimate $K_d$, using Equation 6.

#### 3.1.3.1 $K_d$ values for Fresh Cement Leaching Scenarios.

For fresh cement, variability in pore water chemistry has little influence on solution composition and the concentration of influent anions (into the steel liners) is controlled by cement leaching and steel corrosion. $K_d$ values for each resin radiolysis scenario are estimated for two steel corrosion scenarios with fresh cement leachate.

1. Carbon steel waste containers corrode per Adler-Flitton et al. (2004, 2011) data. Under this scenario, pH declines to about 8.2 and the solution strips enough CO2 out of the vault gas to balance the cationic charge of Na+ and K+ with carbonate ions. Total anion concentration is estimated to be approximately 1,100 meq/L.
    - *No resin degradation*. The exchange capacity is 1.1 meq/cc and $K_d$ is 0 mL/g.
    - *Resins degrade; resin-IEC is calculated over a time period of 0 to 1,500 years.* The median exchange capacity is 1.0 meq/cc and $K_d$ is 0 mL/g.
    - *Resins degrade; resin-IEC is calculated over a time period of 1,500 to 5,000 years.* The median exchange capacity is 0.8 meq/cc and $K_d$ is 0 mL/g.
    - *Resins degrade; resin-IEC is calculated over a time period of 5,000 to 10,000 years*. The median exchange capacity is 0.5 meq/cc and $K_d$ is 0 mL/g.

- *Resins are exposed to radiation from activated metals.* Ion-exchange capacity is 0 meq/cc and $K_d$ is 0 ml/g.

2. *Corrosion is inhibited by high pH. Carbon steel waste containers corrode 100 to 1,000 times more slowly than per Adler-Flitton et al. (2004, 2011) data*. Under this scenario, the high pH inhibits corrosion of waste containers and the system is dominated by OH- and silica anions leached from cement. Total anion concentration is estimated to be approximately 930 to 940 meq/L.

   - *No resin degradation*. The exchange capacity is 1.1 meq/cc and $K_d$ is 0.08 mL/g.
   - *Resins degrade; resin-IEC is calculated over a time period of 0 to 1,500 years*. The median exchange capacity is 1.0 meq/cc and $K_d$ is 0.05 mL/g.
   - *Resins degrade; resin-IEC is calculated over a time period of 1,500 to 5,000 years*. The median exchange capacity is 0.8 meq/cc and $K_d$ is 0 mL/g.
   - *Resins degrade; resin-IEC is calculated over a time period of 5,000 to 10,000 years*. The median exchange capacity is 0.5 meq/cc and $K_d$ is 0 mL/g.
   - *Resins are exposed to radiation from activated metals.* Ion-exchange capacity is 0 meq/cc and $K_d$ is 0 ml/g.

#### 3.1.3.2 $K_d$ values for Mature Cement Leaching Scenarios.

For mature cement, the influent anion concentration into the waste containers is more strongly impacted by variability in the composition of RH-LLW alluvium water. This is because geochemical reactions with mature cement release fewer ions into the solution, yielding more impact from the native solution. $K_d$ values for each resin radiolysis scenario are estimated for two steel corrosion scenarios with mature cement leachate.

1. *Carbon steel waste containers corrode per Adler-Flitton et al. (2004, 2011) data:* Under this scenario, pH declines to about 6.3, anion concentrations are split between carbonates and hydroxides, and total anion charge ranges from 30 to 40 meq/L.

   - *No resin degradation*. The exchange capacity is 1.1 meq/cc and $K_d$ ranges from 13 to 18 mL/g.
   - *Resins degrade; resin-IEC is calculated over a time period of 0 to 1,500 years*. The median exchange capacity is 1.0 meq/cc and $K_d$ ranges from 12 to 16 mL/g.
   - *Resins degrade; resin-IEC is calculated over a time period of 1,500 to 5,000 years*. The median exchange capacity is 0.8 meq/cc and $K_d$ ranges from 9 to 13 mL/g.
   - *Resins degrade; resin-IEC is calculated over a time period of 5,000 to 10,000 years*. The median exchange capacity is 0.5 meq/cc and $K_d$ ranges from 6 to 8 mL/g.
   - *Resins are exposed to radiation from activated metals.* Ion-exchange capacity is 0 meq/cc and $K_d$ is 0 ml/g.

2. *Corrosion is inhibited by high pH. Carbon steel waste containers corrode 100 to 1,000 times more slowly than per Adler-Flitton et al. (2004, 2011) data:* Here, pH is similar to the prior scenario, but reduced corrosion limits anion charge concentration to 20 to 25 meq/L.

   - *No resin degradation*. The exchange capacity is 1.1 meq/cc and $K_d$ ranges from 21 to 24 mL/g.
   - *Resins degrade; resin-IEC is calculated over a time period of 0 to 1,500 years*. The median exchange capacity is 1.0 meq/cc and $K_d$ ranges from 19 to 21 mL/g.
   - *Resins degrade; resin-IEC is calculated over a time period of 1,500 to 5,000 years*. The median exchange capacity is 0.8 meq/cc and $K_d$ is ranges from 15 to 17 mL/g.
   - *Resins degrade; resin-IEC is calculated over a time period of 5,000 to 10,000 years*. The median exchange capacity is 0.5 meq/cc and $K_d$ ranges from 9 to 11 mL/g.
   - *Resins are exposed to radiation from activated metals.* Ion-exchange capacity is 0 meq/cc and $K_d$ is 0 ml/g

### 3.1.4 Summary and $K_d$ Recommendation for Resins

The prior analysis indicates that, if a fresh cement leaching scenario is used, then all corrosion scenarios yield the same $K_d$. $K_d$ will range from 0 to 0.1 mL/g under initial conditions and be effectively 0 mL/g for all subsequent time periods. Consequently, if leaching of fresh cement is assumed, then a $K_d$ of 0 mL/g should be used for release of iodine and technetium from anion-exchange resins.

If a mature cement leaching scenario is used, then pH is lower and there is less inhibition of corrosion. This reduces the certainty that the $K_d$ values derived from inhibited-corrosion scenarios are more accurate than those derived directly from the data of Adler-Flitton et al. (2004, 2011). Consequently, for mature cement, this analysis recommends that the lower $K_d$ ranges be used if a mature-cement leaching scenario is employed. Furthermore, for mature cement scenarios, $K_d$ depends on both the resin degradation scenario and corrosion scenario. $K_d$ is lower under the more aggressive corrosion scenario and $K_d$ values decrease with increasing resin degradation. Consequently, aggressive resin degradation scenarios under more aggressive corrosion scenarios will be more conservative and should provide greater certainty to bounding calculations. Furthermore, because radiolytic degradation of anion-exchange resins will release byproducts that enhance steel corrosion (Pillay 1986a, Gangwer and Pillay 1982), the aggressive corrosion scenario should be adopted for mature cement. Based on these arguments, this analysis recommends $K_d$ values based on corrosion as per Adler-Flitton and resin degradation scenarios for time periods after more than 50% of steel liners are anticipated to have corroded (e.g., greater than 1,500 years). The following four values are considered to be technically defensible.

1. *Baseline performance.* This value corresponds to a scenario where resins do not degrade before they are exposed to leachate from mature cement. Under this case, $K_d$ is likely to range from 13 to 18 mL/g; and the lower value of 13 mL/g is recommended.
2. *Most likely.* This value corresponds to an aggressive resin degradation scenario with a median resin-IEC calculated over the time period between 1,500 and 5,000 years, when over 50% of the steel liners have likely corroded and most release is anticipated to occur. Under this case, the minimum $K_d$ is likely to range from 9 to 13 mL/g; and the lower value of 9 mL/g is recommended.
3. *Reasonably conservative.* This value corresponds to an aggressive resin degradation scenario with a median resin-IEC calculated over the time period between 5,000 and 10,000 years, when all steel liners have likely corroded. It also corresponds to a scenario where steel liners corrode more slowly than anticipated. Under this case, the minimum $K_d$ is likely to range from 6 to 8 mL/g; and the lower value of 6 mL/g is recommended.
4. *Extremely conservative.* This value corresponds to a catastrophic failure scenario, where either leachate from fresh cement enters the waste containers, most resins are exposed to radiation from activated metals, or some combination of these two failure mechanisms occurs. Under this case, either the resins exchange capacity is exhausted or fresh cement leachate overwhelms the resins ability to chemically bind technetium and iodine. For this scenario, a $K_d$ value of 0.0 mL/g is recommended.

Overall, assuming leaching of mature cement provides a more reasonable bounding condition than assuming leaching of fresh cement. This judgment is based on the following arguments:

1. *Cement leachate chemistry* — Prior calculations suggested that if the entire volume of cement has to equilibrate with infiltrating water, then insufficient water will pass through the vault to degrade the cement from fresh to mature or degraded states. Field studies have indicated that the surfaces of cement degrade much more quickly than bulk cement because transport of high pH solutions from cement pores to the exposed surfaces that adjoin transport pathways is limited by diffusion. Given the long-time periods of interest and the RH-LLW vault environment, it is likely that the solutions that move through fissures in the cement or condense on the bottom of the vault's ceiling (and drip onto steel liners) and that they would reflect the composition of mature or degraded cement. It is likely that

the majority of solution mass that encounters the steel liners will be more reflective of mature or degraded cement than of fresh cement.

2. *Corrosion of external surfaces of steel liners* — If fresh cement leaching controls the composition of solution (pH 12 to 14), then the external surfaces of the liners should corrode very slowly and almost all meaningful corrosion would occur on internal surfaces. If mature or degraded cement leaching controls the composition of solution that encounters the liners (pH 6 to 10), then the external surfaces would corrode at rates approaching the CPP-749 (INL 2009) values or buried in soil values of Adler-Flitton (2004, 2011). Corrosion of external surfaces will proceed more quickly in the presence of mature or degraded cement leachate; it is more likely that these lower ionic strength waters will encounter the resins.

Assuming that leachate from mature cement encounters the resins is the most reasonable and technically defendable scenario for all cases where resin containers are interred with other resin containers. Fresh cement leachate is likely to encounter the resins only under scenarios where steel liners are either (1) faulty, (2) physically damaged during internment, or (3) been fully corroded from corrosion processes occurring at internal surfaces. These scenarios provide an implausible worst case; therefore, assuming a $K_d$ for leaching of fresh cement (0 mL/g) provides a bounding condition for the worst groundwater release that could conceivably occur. It is more reasonable to assume that mature or degraded cement leachate will corrode through the containers and come into contact with the resins. This would result in a $K_d$ of 6 to 13 mL/g, depending on the resin degradation, corrosion scenario, and time period in question. The time period of 5,000 to 10,000 years is judged to be reasonably conservative and provide the most reliable bounding conditions. For this time period, the minimum $K_d$ should range from 6 to 8 mL/g and the lowest value in the range (6.0 mL/g) is recommended. The fresh cement $K_d$ (0 mL/g) would only be appropriate for worst case bounding scenarios where the resin's ability to bind radionuclides may be compromised by faulty facility design, excessive internal corrosion, or poor facility operating procedures.

Finally, note that the relative simplicity of the cement model employed here neglects the impacts of dissolution and precipitation of ettringite and monosulfate on solution composition. Inclusion of these minerals into the cement model may elevate predicted $SO_4^{-2}$ concentrations, increase total anion charge, and decrease the release $K_d$ from anion resins. This effect will be negligible for fresh cement, but could be significant for mature cement. Thus, if mature cement scenarios are to be used, additional investigations should be conducted with a more advanced cement chemistry model. Phase transformations between ettringite and monosulfate can be complex and kinetically controlled rather than thermodynamically controlled. Therefore, if such work is done, experimental data with the cement mixture planned for the RH-LLW facility should be gathered. Such experiments and advanced modeling are beyond the scope of this investigation of likely conservative $K_d$ values.

## 3.2 Distribution Coefficient Values for Cement within the Vault

Depending on infiltration rates, some radionuclides may infiltrate into the floor of the cement vault before reaching the drainage holes in the bottom of the vault and infiltrating into the RH-LLW vault underlayment. Additionally, the concrete will decompose into a crushed cement/sand mixture over the life cycle of the facility, allowing more infiltration to pass through cement materials. At a minimum, some radionuclides may precipitate as hydroxide minerals on the surface of the vault due to solubility limits at elevated pH. The current transport model does not account for these interactions, which may provide for a chemical barrier to transport of radionuclides.

This section will provide a brief summary of likely $K_d$ values for radionuclides interacting with cement minerals. The selected radionuclides, shown in Table 13, were identified in the performance assessment (DOE-ID 2010) through a screening analysis as the radionuclides with the greatest potential to impact the groundwater all-pathways dose. The selection of $K_d$ values is based on availability of

comprehensive analyses of prior studies for the given radionuclides, with supporting calculations relevant to a cement repository environment.

The two best summaries of estimated $K_d$ values for radionuclides in vault environments come from Wang et al. (2009) and Krupka and Serne (1998), who combined literature reviews and modeling studies to estimate conservative $K_d$ values for radionuclides in a cement repository environment. Their analysis provides $K_d$ estimates for oxidizing and reducing conditions for three repository environments that correspond to stages of cement degradation shown in Figure 2: fresh cement (KOH/NaOH controlled), mature cement (portlandite controlled), and degraded cement (CSH controlled). In general, the $K_d$ values recommended by Krupka and Serne (1998) were derived by calculating the aqueous solubility of the analyzed radionuclides in the different vault environments, while accounting for pH, pe, and ionic strength. Literature studies were used as a guide to establish equilibrium phases for the calculations and as a source of data from which to compare experimental results with modeling computations. Given the comprehensiveness of the analysis done by Wang et al. (2009) and Krupka and Serne (1998), and the general consistency between their model results for pore water chemistry in a cement environment similar to that employed by this study, there is no strong reason not to adopt the $K_d$ values they recommended. Consequently, their values for fresh cement and mature cement are recommended as provided. These values are summarized in Table 13.

Table 13. Estimated distribution coefficient values for contaminants of concern in cement environments, adopted from Krupka and Serne (1998) or Wang et al. (2009), as available. For cases where data are not available for radionuclide contaminants of concern for the remote-handled low-level facility, estimates are provided. Note that given values are recommended as "best estimate" and not as "conservative."

| | | $K_d$ for Fresh Cement (mL/g) | | $K_d$ for Mature Cement (mL/g) | | $K_d$ for Degraded Cement (mL/g) | | |
|---|---|---|---|---|---|---|---|---|
| Radionuclide | Charge | Oxic | Reducing | Oxic | Reducing | Oxic | Reducing | Reference |
| Ac-227 | cation | — | — | 5,000 | 5,000 | — | — | Initial Estimate (see text) |
| C-14 | anion | 2,000 | 2,000 | 5,000 | 5,000 | 2,000 | 2,000 | Wang et al. (2009) |
| Cl-36 | anion | 20 | 20 | 50 | 50 | 20 | 20 | Wang et al. (2009) |
| H-3 | cation | 0 | 0 | 0 | 0 | 0 | 0 | Wang et al. (2009) (with notes in text) |
| I-129 | anion | 1 | 1 | 10 | 10 | 1 | 1 | Wang et al. (2009) |
| Mo-93 | anion | 0 | 0 | 0 | 0 | 0 | 0 | Initial Estimate (see text) |
| Nb-94 | cation | 50,000 | 50,000 | 50,000 | 50,000 | 50,000 | 50,000 | Wang et al. (2009) |
| Ni-59 | cation | 65 | 65 | 400 | 400 | 400 | 400 | Wang et al. (2009) |
| Np-237 | cation | 2,000 | 30,000 | 2,000 | 30,000 | 200 | 30,000 | Krupka and Serne (1998) for oxidizing, Wang et al. (2009) for reducing |
| Pb-210 | cation | — | — | 500 | 500 | — | — | Initial Estimate (see text) |
| Plutonium (multiple) | cation | 2,000 | 5,000 | 30,000 | 30,000 | 30,000 | 30,000 | Wang et al. (2009) |
| Protactinium (multiple) | cation | 10,000 | 30,000 | 10,000 | 30,000 | 10,000 | 30,000 | Wang et al. (2009) (with notes in text) |
| Radium (multiple) | cation | 300 | 300 | 100 | 100 | 800 | 800 | Wang et al. (2009) |
| Sr-90 | cation | 100 | 100 | 30 | 30 | 100 | 100 | Wang et al. (2009) |
| Tc-99 | anion | 0 | 3,000 | 0 | 3,000 | 0 | 3,000 | Wang et al. (2009) |
| Thorium (multiple) | cation | 30,000 | 30,000 | 30,000 | 30,000 | 30,000 | 30,000 | Wang et al. (2009) |
| Uranium (multiple) | cation | 2,000 | 30,000 | 30,000 | 30,000 | 30,000 | 30,000 | Wang et al. (2009) |

Neither Wang et al. (2009) nor Krupka and Serne (1998) provided $K_d$ values for all radionuclides of concern within the RH-LLW facility and additional estimates are needed in order to evaluate the potential for the cement floor to act as a barrier to radionuclide transport. These estimates should be developed using the same method used by these prior studies, whereby literature review and solubility calculations are used to provide a conservative estimate that is appropriate to the vault environment. Providing this review is beyond the scope of this document, as the current design features for the RH-LLW facility do not provide a basis whereby a conservative estimate can be made that includes the cement floor as a barrier to radionuclide transport. However, it is within the scope of this document to provide rough estimates that can be used to evaluate the potential utility of conducting further investigations. These estimates are presented in the following subsections, with Section 3.2.1 dealing with radionuclides anticipated to have a $K_d$ of approximately 0 and Section 3.2.2 dealing with radionuclides anticipated to have a non-zero $K_d$.

### 3.2.1 Tritium and Molybdenum-93 Sorption onto Cement

Tritium is a conservative tracer used to track water movement. Model calculations do not suggest that elevated pH should retard the movement of tritiated water; therefore, its $K_d$ should be zero. A number of studies suggest that diffusion and imbibition of tritiated water into cement pores controls transport, with isotope exchange reactions acting to absorb tritium that permeates into cement pores (Eicholz et al. 1989, Furuichi et al. 2007, Hochel and Clark 2002). These studies suggest that tritium can be transported through concrete pores, but do not provide retention factors or $K_d$ values that can be used to calculate a $K_d$ for aqueous tritium transport across a cement barrier. Therefore, while there is evidence to suggest that tritium sorption to concrete can retard transport, there is not sufficient data to recommend a non-zero $K_d$ value for groundwater transport of aqueous tritium. This study concurs with Wang et al. (2009) and recommends a $K_d$ of 0 for tritium transport in the vault interior.

Investigations of molybdenum sorption to 32 soil types have indicated that molybdenum sorption is minimal above pH 8, with adsorbed concentrations typically declining to less than 1% of total molybdenum as pH rises above 12 (Goldberg et al. 2002). This equates to a $K_d$ of less than 0.01. Of all 32 soils tested, only one soil had appreciable molybdenum sorption above pH 10 to 12. Carroll et al. (2006) report that molybdenum sorption is minimal above pH 8, though a $CaMoO_4$ precipitate can form if Ca concentrations are high enough. Surfaces that strongly adsorb anions can adsorb the $MoO_4^{2-}$ anions that occur at a pH greater than 4. In a solution that had about 1 mM $Ca^2$ and about 0.15 mM $Mg^{2+}$, Carroll et al. (2006) predicted that approximately 100% of the total molybdenum existed as aqueous species at pH greater than 5. Sorption experiments revealed a $K_d$ of approximately 0.3 at pH 8, which is consistent with the work of Goldberg et al. (2002). Based on these literature reports, this study recommends a $K_d$ value of 0 for Mo-93 in the high pH vault environment.

### 3.2.2 Actinium, Protactinium, and Lead Sorption onto Cement

Actinium, protactinium, and lead are all metallic elements that react to form hydroxide precipitates, with the extent of precipitation increasing with pH. Therefore, they should have a high $K_d$ on cement. Kaplan (2005) estimates that actinium and protactinium have a $K_d$ of 5,000 in oxidizing and reducing cementitious grouts used for waste stabilization at the Savannah River Site. Wang et al. (2009) provide higher estimates for protactinium, and their recommendations are adopted. Lead is estimated to have a $K_d$ of 500 under similar conditions. Kaplan's estimates for actinium are based on data from McDowell et al. (2000) on the $K_d$ for americium in the +3 valence state (e.g., $Am^{III}$), using $Am^{III}$ as an analogue. Estimates for lead are presented as reported by McDowell et al. (2000). It is unclear if the cementitious grouts used at the Savannah River Site have a geochemistry that is analogous to what is expected for the floor of the RH-LLW vault; but they do provide a useful reference point. Given the current state of knowledge, the $K_d$ values recommended by Kaplan (2005) and McDowell et al. (2000) for lead sorption to the cementitious grouts at the Savannah River Site also are recommended for cement in the RH-LLW vault.

## 3.3 Distribution Coefficient Values for the Vault Underlayment not Impacted by Cement Leachate

As discussed in Section 2.6, a sand/gravel underlayment (Zone 6 in Figure 3) will be emplaced under the vault system and will be impacted by cement water and by alluvium water. The sand/gravel underlayment may be constructed of INL alluvial materials. However, to be conservative, this analysis assumes that the underlayment will consist of less adsorptive sands, rather than the more adsorptive native alluvium material. $K_d$ values that previously have been reported for radionuclide sorption to sandy sediment in solutions comparable to native INL alluvium water are provided in Table 14. A recommended conservative value to use for the RH-LLW performance assessment also is included. In all cases, the recommended value is the lowest reported in the literature. These values may be overly conservative, but are reasonable considering the amount of data available. The potential impact of cement leachate from the RH-LLW vault on radionuclide sorption to this sandy sediment is discussed in Section 3.5.

Table 14. Distribution coefficient values for radionuclide sorption to sand and gravel sediment in the vault underlayment. Distribution coefficient values for sand are based on measurements made at Pacific Northwest National Laboratory and Savannah River Site.

| | $K_d$ for Sandy Sediment, Native Water (mL/g) | | | | Recommended conservative $K_d$ value for RH-LLW underlayment (natural alluvium water) |
|---|---|---|---|---|---|
| Radionuclide | Best $K_d$ for non-impacted far-field sand (Cantrell et al. 2007) | Conservative, far-field sand (Cantrell et al. 2007) | Sand sediment (Cantrell et al. 2008) | Sandy SRS sediment Kaplan (2010) | |
| Ac-227 | 300 | 60 | — | 1,100 | 60 |
| C-14 | 5 | 0.5 | 0 | 10 | 0 |
| Cl-36 | 0 | 0 | — | 0 | 0 |
| H-3 | 0 | 0 | 0 | 0 | 0 |
| I-129 | 0.25 | 0 | 0 | 0.3 | 0 |
| Mo-93 | — | 1 | — | 1,000 | 1 |
| Nb-94 | — | — | — | 0 | 0 |
| Ni-59 | 300 | 50 | 50 | 7 | 7 |
| Np-237 | 15 | 2 | 2 | 3 | 2 |
| Pb-210 | 10,000 | 8,000 | 10 | 2,000 | 10 |
| Plutonium (multiple) | 150 | 50 | 200 | 16 | 16 |
| Protactinium (multiple) | — | — | — | 3 | 3 |
| Radium (multiple) | 14 | 5 | — | 5 | 5 |
| Sr-90 | 14 | 5 | 10 | 5 | 5 |
| Tc-99 | 0 | 0 | 0 | 0.6 | 0 |
| Thorium (multiple) | 1,000 | 40 | — | 900 | 40 |
| Uranium (multiple) | 1.0 | 0.2 | 0.2 | 200 | 0.2 |

## 3.4 Distribution Coefficient Values for Alluvium Sediment Not Impacted by Cement Leachate

A number of prior performance assessments and composite analyses performed at INL have utilized $K_d$ values to describe contaminant sorption to INL alluvium and interbed sediment. Rood and Magnuson (2009) provide a summary of $K_d$ values previously used for performance assessments and composite analyses at the INL site. The Idaho Cleanup Project has provided a similar summary specifically for RWMC (Idaho Cleanup Project 2007). The basis for the $K_d$ selections appears to come predominantly

from four documents: (1) a 1990 journal article by Sheppard and Thibault (1990) on "default partition (distribution) coefficients" that can be used if site-specific data are not available, (2) a second addendum to the work plan for the Operable Unit 7-13/14 waste area group (Holdren and Broomfield 2004), and (3) a guidance document for assessing "low probability hazard sites at INL" published by DOE Idaho Operations Office (DOE 1994), and (4) more recently, Cahn et al. (2006) provide a detailed derivation of their $K_d$ values in Appendix D of the baseline risk assessment for Operable Unit 3/14 (Idaho Nuclear Technology and Engineering Center facility). The DOE guidance document (DOE 1994) specifies that when INL-specific values are not available, $K_d$ values measured for basalt or interbed minerals from the Hanford site (Kelmers 1984) or 1990 values from Sheppard and Thibault (1990) can be used.

### 3.4.1 Summary of Results from Prior Studies

With the exception of Cahn et al. (2006), most $K_d$ values that prior reports have deemed applicable as conservative estimates for radionuclide transport in INL sediment are based on the work of Sheppard and Thibault (1990). Therefore, it is useful to more closely examine the applicability of these "default" values to the RH-LLW alluvium, including the following in particular:

1. Sheppard and Thibault (1990) classify their sand and loam on the basis of sediment grain size rather than mineralogy, with the grain size distribution of INL sediment generally corresponding to the sand or loam classifications. However, prior studies relating Kd values to sediment properties at INL specifically conclude that Kd is primarily related to CEC and mineralogy and only secondarily related to grain size (Leecaster and Hull 2003).
2. Sheppard and Thibault (1990) did not report the mineralogy of the default sediment they used, and many of their default Kd values are derived indirectly from reported soil-to-plant ratios rather than direct measurements.
3. The default values from Sheppard and Thibault (1990) do not consider the effects of changing water chemistry. However, studies of $Sr^{2+}$ $K_d$ in INL sediment have clearly demonstrated that extremes in solution chemistry can greatly alter $K_d$ values (Hull and Schafer 2008).

As a result of these considerations, the method of estimating $K_d$ on the basis of how closely the grain size distribution of INL sediment corresponds with a value from Sheppard and Thibault (1990) is not firmly based in scientific theory. There are alternative methods for $K_d$ estimation that are more scientifically robust. This stated, it should be noted that a number of site-specific studies conducted under steady-state conditions with INL sediment have generally confirmed that a $K_d$ from either a sand or a loam (Sheppard and Thibault 1990) is reasonable to use as a conservative estimate for radionuclide transport in INL alluvium sediment under steady-state conditions. Therefore, while these default values should not be adopted without careful consideration and confirmatory analyses, they do provide a guide that can be useful if (1) no other data are available for a given radionuclide and (2) they are consistent with available confirmatory data regarding the sorption of the specific radionuclide to comparable sediment under anticipated geochemical conditions. A comparison of the default values from Sheppard and Thibault (1990) with site-specific studies and recommended $K_d$ values for performance assessments and composite analyses previously performed at INL are presented in Table 15.

Table 15. Distribution coefficient values (mL/g) previously recommended for Idaho National Laboratory performance assessments, potentially applicable to the remote-handled low-level waste alluvium, and recommended distribution coefficient values for remote-handled low-level waste alluvium under natural (undisturbed) conditions.

| | Prior INL Values (Rood and Magnuson 2009) | Range and (Recommended) Kd values for Operable Unit 3/14 (Cahn et al., 2006) | Sand (Sheppard and Thibault 1990) | Loam (Sheppard and Thibault 1990) | Site-specific Measurements | Reference for Site-Specific measurements of Kd on INL Sediment | Recommended Kd for Alluvium at RH-LLW Facility |
|---|---|---|---|---|---|---|---|
| Ac-227 | 225–450 | — | 450 | 1,500 | — | — | 300 |
| C-14 | 0–5 | 0.5–2.8 (1.6) | 5 | 20 | 0.5–2.4 | Plummer et al. (2004), Fox et al. (2004) | 0.5 (INL data) |
| Cl-36 | 0 | — | — | — | — | — | 0 |
| H-3 | 0 | — | — | — | 0.04–0.1 | Fox et al. (2004) | 0 |
| I-129 | 0 | 0.04–8.7 (1.5) | 1 | 5 | — | — | 3.8–6.1 (literature value) |
| Mo-93 | 10 | — | 10 | 125 | — | — | 10 |
| Nb-94 | 500 | — | 160 | 550 | — | — | 160 |
| Ni-59 | 100 | — | 400 | 300 | -- | — | 100 |
| Np-237 | 23 | 0.1–60 (2) | 5 | 25 | Short-contact: 40–500<br>Long-contact; 0.02–250 (median about 35) | Mincher et al. (2003), Leecaster and Hull (2003), Ayaz et al. (2003), Dicke (1997), Grossman et al. (2001) | 18 (INL data) |
| Pb-210 | 100–270 | — | 270 | 16,000 | — | — | 270 |
| Plutonium (multiple) | 140–2,500 (recommend 2,500) | 96–12,712 (1,000) | 550 | 1,200 | Short-contact: 14–650<br>Long-contact; 140–22,000 (median about 2,680) | Mincher et al. (2003), Miner et al. (1982), Dicke (1997), Navratil (1997), Newman (1996), Fjeld et al. (2000, 2001), Mincher (unpublished data, 2004) | 1,140 (INL data) |
| Protactinium (multiple) | 8–550 | — | 550 | 1,800 | — | — | 550 |
| Radium (multiple) | 100-575 | — | 500 | 36,000 | — | — | 500 |
| Sr-90 | 18 | 8–20 (12) | 15 | 20 | Perturbed alluvium: 0.01–90 (typical 11)<br>Steady state: 5–1,000 (typical range 34–275) | del Debbio and Thomas (1989), Mincher et al. (2003), Hull and Schafer (2005, 2008), Liszewski et al. (1997, 1998) | 11-22 (INL data) |
| Tc-99 | 0–0.2 | -0.1–1.4 (0) | 0.1 | 0.1 | 0 | del Debbio and Thomas (1989) | 0.1 |
| Thorium (multiple) | 100–500 | — | 3,200 | 3,300 | — | — | 500 |

Table 15. (continued).

| | Prior INL Values (Rood and Magnuson 2009) | Range and (Recommended) Kd values for Operable Unit 3/14 (Cahn et al., 2006) | Sand (Sheppard and Thibault 1990) | Loam (Sheppard and Thibault 1990) | Site-specific Measurements | Reference for Site-Specific measurements of Kd on INL Sediment | Recommended Kd for Alluvium at RH-LLW Facility |
|---|---|---|---|---|---|---|---|
| Uranium (multiple) | 6–15.4 | 0.12–12 (1.6) | 35 | 15 | 3–79 (median about 21) | Leecaster and Hull (2003), Dicke (1997), Ayaz et al. (2003), Fjeld et al. (2000, 2001), Hull et al. (2002), Hull et al. (2004) | 10 (INL data) |

### 3.4.2 Justification for Selection of Distribution Coefficients for Radionuclides of Concern Where There are No Site-Specific Data

For cases where there are no site-specific data, this report generally recommends values where there is the greatest agreement between prior INL recommendations and default $K_d$ values proposed by Sheppard and Thibault (1990) for sand. The sand values from Sheppard and Thibault (1990) are typically the lowest (e.g., most conservative) of all the values reported by these researchers, and the grain size distribution most closely matches that of INL. However, in four cases, this analysis recommends different $K_d$ values than the sand values suggested by Sheppard and Thibault (1990): actinium, iodine, nickel, and thorium. For actinium, we adopt the "recommended far-field non-impacted sand" value from Cantrell et al. (2007), as summarized in Column 2 of Table 13. This value is intermediate between the range recommended by Rood and Magnuson (2009) and the sand value from Sheppard and Thibault (1990). For nickel and thorium, prior transport studies conducted at INL have used $K_d$ values significantly lower than the sand $K_d$ values provided by Sheppard and Thibault (1990). No justification is given for this decision in the reports where the $K_d$ values are cited, but it must be assumed that the prior analysts based their decision to use lower $K_d$ values on analyses conducted during the course of their work. Thus, in order to be conservative, these lower estimates are adopted for nickel and thorium. For nickel, only one value (100) is given, and that value is adopted. For thorium, a range is given (100 to 500). The value of 500 is adopted, as that is the $K_d$ used for RWMC (Idaho Cleanup Project 2007) and is closest to the sand $K_d$ recommended by Sheppard and Thibault (1990).

For iodine, this analysis recommends a $K_d$ significantly larger than previously recommended for INL or for default sand sediment. It also is larger than previously recommended for default loam sediment. The justification for this selection comes from a review of the literature on iodine chemistry in natural systems. Prior recommendations for iodine $K_d$ in INL sediment range from 0 to 8.7, with the most common recommended value of 1.0 to 1.5 being based on the "iodine sorption to sand" value proposed by Sheppard and Thibault (1990). This earlier work is based on literature surveys of pre-1990 studies and not direct measurements that (1) take advantage of modern analytical capabilities and (2) account for the impacts of iodine chemical speciation in different sediment types. Hu et al. (2005) evaluated the sorption and transport of iodine in sediment from the Hanford and Savannah River sites and also provides a nice review of recent advances in our understanding of iodine sorption and transport in natural environments. A brief summary of their key points is provided here. In general, the fate and transport of iodine in aqueous environments is dictated by its chemical speciation. Iodide ($I^-$) is more mobile and more prevalent in reducing and moderately oxidizing environments. Iodate ($IO_3^-$) is less mobile and more prevalent in strongly oxidizing conditions. However, as long as oxygen is present, both species commonly coexist. Iodine is readily incorporated into organic matter by both biotic and abiotic processes, and organic iodine species can represent a significant fraction of total iodine. For example, methyl iodide is a gaseous form that can comprise up to 50% of total iodine in river, ocean, and estuarine systems. Coexistence of these different species of iodine has been reported in a number of environments, and thus

total iodine in any given environment is likely to be a mix of $I^-$, $IO_3^{2-}$, and organic iodine. The $K_d$ of all iodine species is known to be highly dependent on iodine mass concentration. Ambient concentrations in radionuclide repositories are typically on the order of $10^{-7}$ to $10^{-8}$ molar, but laboratory experiments are typically conducted at concentrations that are 10 to 10,000 times higher (e.g., $10^{-4}$ to $10^{-6}$ molar). Therefore, the sediment chemistry that controls iodine sorption under ambient conditions is very different from that measured in laboratory experiments. This artificially reduces $K_d$ values (Kaplan et al. 2010; Zhang et al., 2010; Schwehr et al., 2009). For example, Schwehr et al. (2009) conducted batch experiments on Savannah River Site sediment at multiple iodide concentrations and found that iodine $K_d$ varied with iodide concentration via an inverse power function. $K_d$ for iodide ($I^{2-}$) at ambient concentrations (e.g., $10^{-7}$ to $10^{-8-}$ molar) was 10 to 30 times higher than at typical experimental concentrations (e.g., $10^{-4}$ to $10^{-6}$ molar), and the mass distribution between iodide, iodiate, and organic iodine moieties also varied with concentration. Thus, $K_d$ values measured at total iodine concentrations required for typical experiments that use mass-based analytical techniques clearly do not reflect actual *in situ* processes, where radioanalytic techniques are needed to measure iodine. Iodine sorption experiments at ambient concentrations have not been conducted for INL sediment; therefore, data are not available for ambient conditions. However, it is clear from literature reports that laboratory studies with elevated iodine levels will underestimate ambient $K_d$, potentially by an order of magnitude (e.g., 10-fold).

Literature reports also indicate that a full description of iodine transport should account for the concentration-dependent sorption parameters of these different species to geologic media, multi-phase transport, and the kinetics of transformation between these different chemical species. Such a model requires extensive experimental work to provide accurate parameters and is beyond the scope of this work. Therefore, this brief review attempts to discern a reasonably conservative $K_d$ for total iodine that is realistic for the RH-LLW alluvium and interbed sediment, given current knowledge of iodine chemistry in INL sediment. All literature reports used for this assessment used mass-based analytical techniques that require artificially high iodine levels and should underestimate $K_d$ at ambient concentrations. Values derived from them should be conservative and bounding for the RH-LLW facility.

Sheppard (2003) used batch sorption experiments to estimate the $K_d$ for sorption of iodine to five different soil types for contact periods of 1-day and 14-days. $K_d$ was higher for long contact time than for short contact time in every case, with the $K_d$ for the long contact time typically being 2 to 60 times greater. Sheppard's 2003 experiments also demonstrated that the iodine $K_d$ for a soil was approximately equal to the weighted average of the $K_d$ of constituent soil types. Therefore, if a soil could be described as 30% Type A, 30% Type B, and 40% Type C; then the $K_d$ would be the weighted average of the $K_d$ for each of these soil types. Of the soil types tested, RH-LLW alluvium sediment most resembles the Milner (2-week $K_d$ = 6.1), Golke (2-week $K_d$ = 140), and Almassippi (2-week $K_d$ = 38) types investigated by Sheppard (2003) on the basis of grain size, iron content, CEC, and organic content. Of the sediment evaluated by Sheppard (2003), the single lowest "long-contact time" iodine $K_d$ of the potentially emulative soil types was the Milner sediment ($K_d$ = 6.1).

With regards to iodine sorption at short contact, Hu et al. (2005) employed column experiments to evaluate iodine sorption to Hanford and Savannah River Site sediment at contact times of approximately 1.5 hours. For Hanford sediment, which is most comparable to RH-LLW alluvium and interbed sediment, observed iodate retention in the sediment columns was 20 to 30% higher than for iodide; iodate reduction to iodide occurred; and some irreversible sorption was observed. Iodine retention factors and the extent of iodate reduction increased with retention time (1.5 hours versus 7.3 hours), and the extent of irreversible sorption increased with decreasing levels of total iodine. Bulk density and sediment porosity for these column experiments were not reported and $K_d$ measurements are not available. However, assuming values that are typical of Hanford sediment (e.g., 35% porosity, 1.5 g/cc bulk density), the reported retention factors at a 1.5-hour contact correspond to short-term contact $K_d$ values of approximately 0.05 for iodide and 0.16 for iodate. Taken together, these values are comparable to the 24-hour contact batch experiments for total iodine sorption of the Milner sediment, as reported by Sheppard (2003).

With regards to long-contact, Kaplan et al. (2000) conducted iodine batch sorption experiments for both (1) a set of sediment collected from the Hanford site, and (2) a range of sediment minerals commonly found in arid sediments of the western United States. All sorption experiments used iodide only (no iodate), were conducted for periods of time ranging from 7 to 350 days using an environmentally relevant concentration of iodine (about 100 micro-Ci/L), had solution conditions comparable to native conditions at Hanford and INL, and employed sediment with a CEC and clay mineral content that is at least 50% lower than for RH-LLW alluvium. Results from these experiments were comparable to what had been reported from prior literature surveys of iodide sorption experiments with Hanford sediment (Kaplan and Serne 1995). $K_d$ values from prior experiments with Hanford sediment ranged from 0.7 to 15 mL/gram, with a mean of 3.1 mL/g. Over all of the measurements conducted during the 250-day tenure of the experiments conducted by Kaplan et. al. (2000), $K_d$ values ranged from 0.07 to 10.6 mL/g, with a mean of 3.85 ±1.03 mL/g. Iodide $K_d$ increased markedly over time, with 1-year experiments yielding mean $K_d$ values that were 125% to 5,000% higher than had been observed at 1-week contact. One-week $K_d$ values ranged from 0 to 2 mL/g, while 350-day $K_d$ values ranged from 4 to 10 mL/g with a mean of about 7 mL/g. Corollary experiments with sediment mineral constituents revealed that iodide primarily adsorbed onto illite surfaces. Native illite had an iodide $K_d$ of about 15 ml/g; while illite that had been treated to remove iron oxides, carbonates, and organic matter had a $K_d$ value of 27.8 mL/g. Sorption to illite was strongly pH dependent, with $K_d$ for "treated" illite ranging from a maximum of 59 mL/g at pH 5.0 to a minimum of 22 mL/g at pH 9.4. Based on these data, Kaplan et al. (2000) concluded that iodide sorption to arid sediment occurred primarily to illites, likely via a mechanism with irreversible sorption to pH-dependent edge sites. The observed increase of iodide sorption over time could potentially be attributable to diffusion-limited access of iodide to reactive edge sites on illite surfaces.

Given the long contact time anticipated in the unsaturated alluvium system at INL, this analysis concludes that the 2-week contact experiments reported by Sheppard (2003) and 250-day contact experiments conducted by Kaplan et al. (2000) are more representative of INL conditions than experiments with shorter contact times. INL sediment has a larger clay mineral content than either the Hanford sediment or the Milner sediment and INL's clay minerals are largely comprised of illite. Consequently, at long contact, RH-LLW alluvium and interbed sediments should sorb iodide more strongly than either the Milner sediment ($K_d$ about 6.1) or Hanford sediment (mean $K_d$ about 7). On the basis of this information, the minimum iodine $K_d$ observed by Sheppard (2003) at 2-week contact time (Milner sediment, $K_d = 6.1$) is recommended as a "most likely" estimate for iodine sorption to native RH-LLW alluvium and interbed sediment.

If greater conservatism is desired, then there are three sets of values that can be used to provide a likely lower bound. First, the mean of all iodine $K_d$ values from Kaplan and Serne (1995) was 3.1 mL/g. Second, the mean of all values for all western sediment over all time periods measured by Kaplan et al. (2000) was 3.85 ±1.03 mL/g. Third, the mean of the 1-year contact experiments with all western sediment conducted by Kaplan et. al. (2000) was 7 mL/g. Together, these experiments yield mean iodine $K_d$ values for sediment comparable to INL alluvium that ranges from a minimum of 2.8 to a maximum of 7 mL/g. The minimum of 2.8 mL/g is the lower bound of the average and standard deviation for all sediment and all time periods considered by Kaplan et al. (2000). This range encompasses the Milner sediment from Sheppard (2003) and all median values from Kaplan et al. (2000) and Kaplan and Serne (1995). Based on these ranges of median values, an iodine $K_d$ of 3.0 mL/g is recommended as "reasonably conservative." This value is the extreme lower bound of the median values from Kaplan et al. (2000), rounded up to the nearest integer value.

### 3.4.3 Justification for Selection of Distribution Coefficients for Radionuclides of Concern Where There are Site-Specific Data

Radionuclides of concern for the RH-LLW facility are given in Tables 13 – 15. Of these nuclides, site-specific studies exist for C-14, H-3, neptunium, plutonium, strontium, and uranium. Tritium, C-14, and uranium transport has been evaluated in a large, meso-scale column reactor packed with INL surficial

sediment from Spreading Area B, a playa southwest of RWMC (Fox et al. 2004, Plummer et al. 2004). This sediment has a grain-size and clay mineral content that is in the middle of the range of what has been observed for all INL interbed sediment, and toward the upper end of what has been observed for interbed sediment at the ATR Complex. In these experiments, the observed $K_d$ ranged from 0.5 to 2.4 for C-14 and from 0.04 to 0.1 for tritium. The recommended conservative $K_d$ values applicable to the ATR interbed sediment are 0.5 for C-14 and 0 for tritium (rounded to 0 from 0.04). These are at the lower range of the measured values.

***3.4.3.1 $K_d$ Values for Neptunium.*** Neptunium sorption has been measured by multiple researchers (Ayaz et al. 2003, Dicke 1997, Grossman et al. 2001, Leecaster and Hull 2003, Mincher et al. 2003). Mincher's experiments at short contact times (less than 2 hours) yielded Freundlich isotherms with derived Kd values ranging from 40 to 50 mL/g. The other researchers employed a combination of batch and column experiments to investigate Np sorption at longer contact times. These experiments generated approximately 54 measurements of Np Kd in INL alluvium and interbed sediment with cation exchange capacities ranging from 3 to 44 meq/ 100 g (median 20 meq/100 g). A histogram of these values is provided in Figure 10. If the range of data presented here are considered in the context of Np geochemistry (e.g., Appendix D of Cahn et al. 2006), then a range of likely values can be derived by scaling the median and confidence intervals of these measurements from the cation exchange capacity (CEC) of experimental sediment down to the expected CEC of RH-LLW alluvium. The expected CEC of RH-LLW alluvium is estimated from available measurements previously made at the ATR Complex (Figure 7), and recent analyses of sediments collected from the proposed site for the RH-LLW facility.

- **Most likely minimum = 11 mL/g.** Value derived by scaling median (35 mL/g) minus the 95% confidence interval for 54 samples (12.7 mL/g) to the ratio of RH-LLW CEC (10 meq/100 g) to experimental CEC (20 meq/100 g). (35-12.7)*(10/20) = 11.
- **Most likely actual = 18 mL/g.** Value derived by scaling median (35 mL/g) to the ratio of RH-LLW CEC (10 meq/100 g) to experimental CEC (20 meq/100 g). (35)*(10/20) = 17.5.
- **Most likely maximum = 24 mL/g.** Value derived by scaling median (35 mL/g) plus the 95% confidence interval for 54 samples (12.7 mL/g) to the ratio of RH-LLW CEC (10 meq/100 g) to experimental CEC (20 meq/100 g). (35+12.7)*(10/20) = 24.

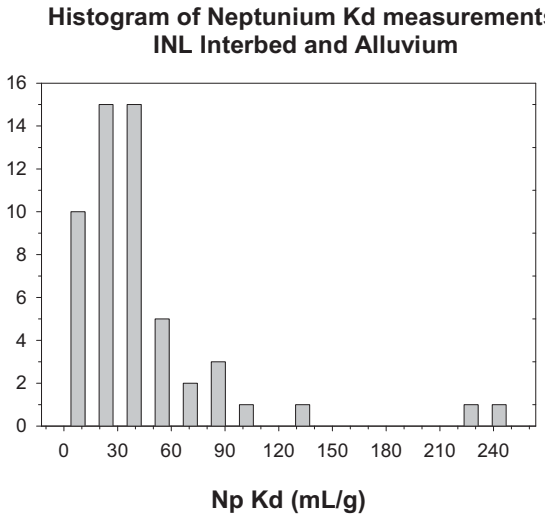


Figure 10. Histogram of measured distribution coefficient values for neptunium sorption to Idaho National Laboratory sediment with cation exchange capacity, ranging from 3 to 44 meq/100 g (median about 20 meq/100 g). Median cation exchange capacity of remote-handled low-level waste alluvium is 10 meq/100 g.

***3.4.3.2 $K_d$ Values for Plutonium.*** Plutonium sorption has been measured by multiple researchers (Dicke 1997, Fjeld et al. 2001, Miner et al. 1982, Newman 1996, Navratil 1997, Mincher et al. 2003). Mincher's experiments at short-contact times (less than 2 hours) yielded Freundlich isotherms, whose derived $K_d$ values ranged from 14 to 650 mL/g. Geochemical modeling conducted in concert with the work of Mincher et al. (2003) demonstrated that multiple sorption processes appeared to be competing and that Pu-239 sorption at a short contact time likely resulted from a combination of the formation of plutonium surface complexes on clay minerals, iron oxide minerals, and precipitation of amorphous $Pu(OH)_4$. As time progressed, these more soluble phases likely hydrolyze to form less soluble $PuO_2(OH)_2$ and $PuO_2$ minerals. This process would lead to higher observed $K_d$ values over time; potentially explaining the discrepancy in observed plutonium $K_d$ values between short-contact experiments and other reports that used longer contact times. When contact time in Mincher's experiments was extended to 2 months, $K_d$ values increased to a range of 1,000 to 10,700 mL/g (Mincher personal communication 2004). Published long-term Pu sorption experiments have generated approximately 30 measurements of Pu $K_d$ in INL alluvium and interbed sediment whose cation exchange capacity is equivalent to that of the RH-LLW sediment.

A histogram of measured plutonium $K_d$ values is provided in Figure 11. Unlike the Np distribution, whose shape is somewhat normal, this distribution is flat and skewed to lower values. Thus, an approach that uses the median and confidence intervals to estimate likely minimum, actual, and maximum values is inappropriate. This skew may arise from how Pu oxidation-reduction chemistry impacts adsorption in INL sediment (e.g., Appendix D of Cahn et al. 2006) or may arise from an experimental artifact. Because the cause is unknown, we have biased our method for deriving most likely $K_d$ values toward the lower end of the distribution.

- **Most likely minimum = 280 mL/g.** Value derived by calculating the median of 50% of all samples that had a $K_d$ within the range of 70 to 700 mL/g. The median of these samples is 280 mL/g. This value was not scaled to CEC.
- **Most likely actual = 1,140 mL/g.** Value derived by calculating the median value of all measurements (2,680) minus the 95% confidence interval for 26 samples (1,540 mL/g). This value is not scaled to CEC.
- **Most likely maximum = 2,680 mL/g.** Value derived by calculating the median value of all measurements. This value is not scaled to CEC.

A number of researchers also have noted the potential for a small fast fraction of plutonium to be transported with a $K_d$ much lower than that of the bulk plutonium. The nature of this fast fraction may arise from either colloidal transport or Pu oxidation-reduction kinetics (Knopp et al. 1999, Fjeld et al. 2001). Experiments by Fjeld et al. (2001) reported that the observed "Pu fast fraction" in his column experiments with INL sediment comprised approximately 1.0 to 2.5% of the total plutonium in his system, and these studies have been used as a basis for evaluating the potential for fast plutonium transport in the buried waste environment at the Radioactive Waste Management Complex (RWMC). However, the chemical impacts of the RH-LLW disposal facility cement vault could impact the potential extent of enhanced plutonium transport through the vault and the underlying media. From existing evidence, we can conclude that only a small fraction, if any, Pu would potentially experience a period of enhanced transport. Given the lack of facility-specific influences on colloidal transport, this analysis recommends evaluating this potential transport pathway via sensitivity analyses.

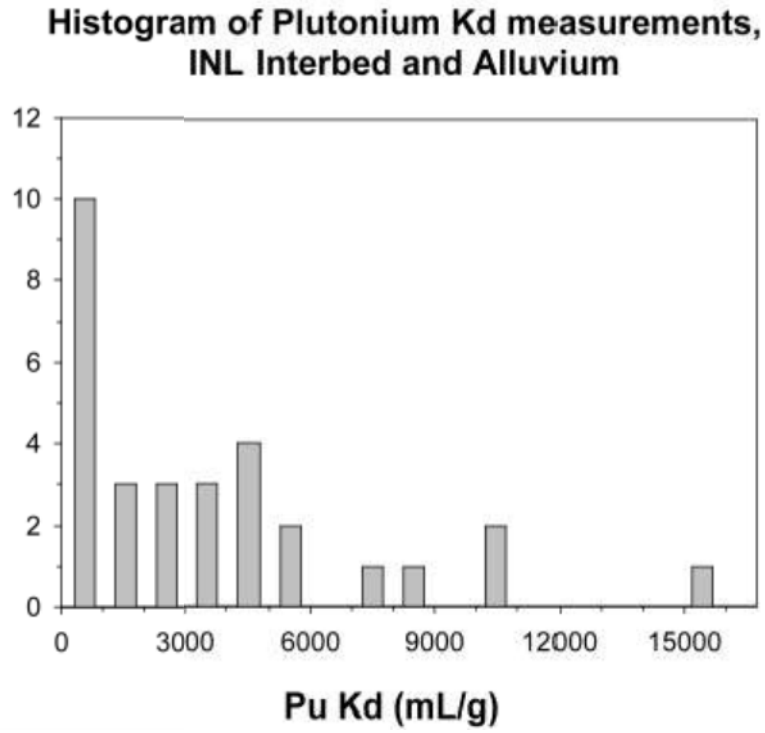


Figure 11. Histogram of measured distribution coefficient values for plutonium sorption to Idaho National Laboratory sediment with cation exchange capacity values approximately equivalent to those in the remote-handled low-level waste alluvium.

***3.4.3.3 $K_d$ Values for Strontium.*** Strontium sorption to INL sediment has been less extensively investigated, and site-specific data is available for studies conducted at the Idaho Nuclear Technology and Engineering Center facility (Hull and Schafer 2008, Hull and Schafer 2005, del Debbio and Thomas 1989, Liszewski et al. 1997, Liszewski et al. 1998). Of all these experiments, only the work of Hull and Schafer (2005) provides corollary CEC values. Even then, CEC values are calculated from ion selectivity coefficients and the solution chemistry reported by prior researchers and not from direct measurements. This report derives Sr $K_d$ values only from sediment where CEC estimates are available (i.e., Hull and Schafer 2005). This approach is conservative because it accounts for CEC and includes a lower bound where the CEC is significantly lower than in sediment at the RH-LLW site. A histogram of these sorption data is provided in Figure 12. The data in the histogram are based on Hull and Schafer (2005), where CEC values are estimated from solution chemistry reported by Liszewski et al. (1997, 1998). As before, most likely minimum, actual, and maximum $K_d$ values can be derived from these data using the median and 95% confidence intervals. Because the CEC of these measurements is lower than the CEC of the RH-LLW alluvium, conservatism is provided by not scaling these $K_d$ measurements to CEC.

- **Most likely minimum = 5 mL/g.** Value derived by calculating median (21.7 mL/g) minus the 95% confidence interval for 21 samples (17.1 mL/g) to yield a value of 4.6 mL/g. This value is not scaled to CEC and lies at the extreme low end of all measurements.
- **Most likely actual = 11 to 22 mL/g.** Lower value from Hull and Schafer (2008). Upper value derived by calculating median. This range of values is not scaled to CEC.
- **Most likely maximum = 39 mL/g.** Derived by calculating median (21.7 mL/g) plus the 95% confidence interval for 21 samples (17.1 mL/g) to yield a value of 38.8 mL/g. Not scaled to CEC.

This study recommends a range of values for the "most likely" $Sr^{2+}$ $K_d$ because (1) $Sr^{2+}$ in INL sediments primarily adsorbs to cation exchange sites in clay minerals in a manner that is sensitive to

changes in solution cation composition, and (2) the major ion composition of the groundwater solution will change as the RH-LLW facility ages (Table 9). The recommendation for the lower bound (11 mL/g) is based on the work of Hull and Schafer (2008), who investigated $Sr^{2+}$ transport in a sediment system where a large pulse of concentrated nitric acid created extreme shifts in solution chemistry (e.g., pH, ionic strength, and cation ratios). Hull and Schafer estimated a $Sr^{2+}$ Kd of 11 mL/g for native alluvium water not impacted by acid. The sediment in their study had a lower mass percentage of fine-grained materials and a CEC that is approximately five times a lower CEC than sediment at the RH-LLW facility. The $Sr^{2+}$ $K_d$ at the RH-LLW facility should not drop below this value. The recommendation for the upper bound (22 mL/g) is based on the calculations of Hull and Schafer (2005), who estimated that the CEC of sediment used in the $Sr^{2+}$ $K_d$ experiments of Liszewski et al. (1997, 1998) ranged from 1.5 to 14.5 meq per 100 g. This CEC value falls within the range measured for surface sediment at the ATR Complex (Figure 7), indicating that sediment at the RH-LLW facility is comparable to those used by Liszewski et al. (1997, 1998).

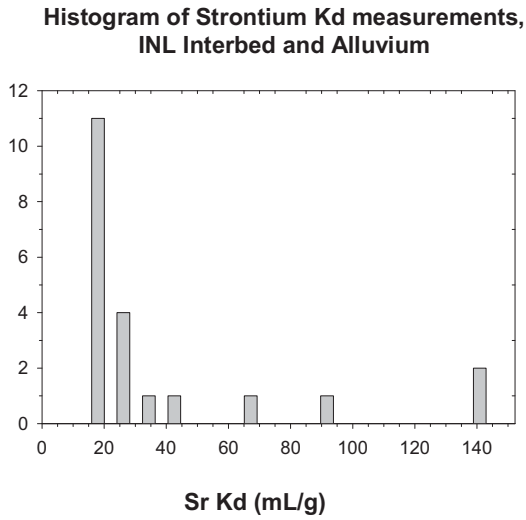


Figure 12. Histogram of measured distribution coefficient values for strontium sorption to Idaho National Laboratory sediment with known cation exchange capacity, ranging from 2 to 14 meq/100 g (median about 2.5 meq/100 g). Median cation exchange capacity of remote-handled low-level waste alluvium is 10 meq/100 g.

The work of Hull and Schafer (2008) also indicate that this range of $K_d$ values (11 to 22 mL/g) should provide a conservative bounding estimate for groundwater transport under the dynamic conditions anticipated for the RH-LLW facility. First, their CEC is lower than at the RH-LLW facility, indicating that baseline $Sr^{2+}$ $K_d$ values at the RH-LLW facility should be higher than reported for the Idaho Nuclear Technology and Engineering Center. Second, Hull and Schafer (2008) report that flushing $Ca^{2+}$ out of a sediment system with $Na^+$ can elevate $Sr^{2+}$ $K_d$. Degradation of fresh cement will release $Na^+$ and $K^+$ into the underlying sediment, flushing a portion of $Ca^{2+}$ off ion-exchange sites before the steel liners begin to corrode. Also, $Ca^{2+}$ concentrations will be suppressed through elevated pH (Table 9). This cation balance could persist for a long time, shifting the system to one comparable to that reported by Hull and Schafer at the Idaho Nuclear Technology and Engineering Center 20 years after the acid release. These elevated values (Hull and Schafer 2008) were universally above 30 mL/g for Idaho Nuclear Technology and Engineering Center sediment that has a lower CEC than at the RH-LLW facility. Finally, the range of recommended values is lower than the range of 34 to 275 reported for INL alluvium by del Debbio and Thomas (1989) and Liszewski et al. (1997 and 1998) and is at the lower end of the range of 5 to 1,000 mL/g reported by Mincher et al. (2004).

Taken together, these arguments indicate that a $Sr^{2+}$ $K_d$ in the range of 11 to 22 mL/g will provide a lower bound for the extent of $Sr^{2+}$ sorption at the RH-LLW facility. The value of 22 mL/g is the most likely lower bound for $Sr^{2+}$ $K_d$ in this sediment, but a value of 11 mL/g is reasonable if a greater degree of conservatism is desired.

***3.4.3.4 $K_d$ Values for Uranium.*** Uranium is the most extensively investigated element in INL sediment, with over 100 batch and column measurements of sorption to and transport through INL sediment available (Ayaz et al. 2003, Dicke 1997, Fjeld et al. 2000, Fjeld et al. 2001, Leecaster and Hull 2003; Hull et al. 2002, Hull et al. 2004). The range of CEC values for uranium measurements on INL sediment is the same as that for Np measurements, and a number of reports discuss how the geochemical factors that control uranium sorption may impact uranium transport in INL sediment. A short introductory summary can be found in Appendix D of Cahn et al. (2006); extensive discussions can be found in these other documents. A histogram of available uranium sorption data to INL sediment is provided in Figure 13. As with Np and Sr, the approach of calculating a median value and 95% confidence intervals is used to estimate the most likely minimum, actual, and maximum uranium $K_d$ values for RH-LLW alluvium sediment, unless there is strong evidence to suggest a more conservative minimum possible value. Also, as with Np, these values are scaled to CEC in order to provide a conservative estimate that is derived from prior geochemical investigations conducted at INL (Leecaster and Hull 2003). Recommended $K_d$ values for uranium sorption to RH-LLW alluvium under natural conditions are as follows.

- **Most likely minimum = 6 mL/g.** Basis is the median of column experiments from Fjeld et al. (2000 and 2001) and unpublished uranium data from mesoscale column reactor experiments for $^{14}C$, $^{3}H$, and uranium transport (Plummer et al. 2004, Fox et al., 2004). These experiments yielded uranium $K_d$ values in the range of 8 to 10 mL/g in sediment that had a CEC of about 16 meq/100 g. When scaled to a CEC of 10 meq/100 g for RH-LLW alluvium, $K_d$ = 10 mL/g*(10/16) = 6.2 mL/g.
- **Most likely actual = 10 mL/g.** Basis for this is the median of all batch experiments (21 mL/g), scaled linearly to CEC. $K_d$ = 21 mL/g *(10/22) = 10 mL/g.
- **Most likely maximum = 11 mL/g.** Basis for this is the median of all batch experiments (21 mL/g) plus 95% confidence interval (2.5), scaled linearly to CEC. $K_d$ = (21 + 2.5) mL/g *(10/22) = 11 mL/g.

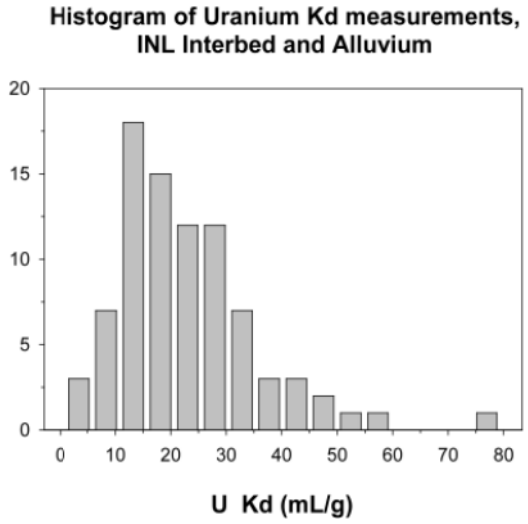


Figure 13. Histogram of measured distribution coefficient values for uranium sorption to Idaho National Laboratory sediment with cation exchange capacity ranging from 3 to 44 meq/100 g. For column experiments, the median cation exchange capacity was 16 meq/100 g, and for batch experiments, the median cation exchange capacity was about 22 meq/100 g. Median cation exchange capacity of the remote-handled low-level waste alluvium is 10 meq/100 g.

## 3.5 Impact of Cement Leachate on Distribution Coefficient Values for the Sand/Gravel Underlayment and Alluvium Sediment

As discussed previously, model calculations of the geochemical environment in the areas beneath the vault (Points #6 and #7 in Figure 3) indicate that the chemistry of the solution will change as the cement degrades, and the impact of this change is dependent on the mixing ratio between water that is in contact with the vault and water that infiltrates in laterally from the surrounding backfill (e.g., Figure 1 and Table 10). This means that $K_d$ will vary with the water infiltration scenario and that a single $K_d$ may not be appropriate for all simulations. Model calculations summarized in Table 10 suggest that the groundwater beneath the RH-LLW vault will have one of five general compositions:

1. Fresh cement – high pH (above 12), high ionic strength (above 1,100), with key parameters not dependent on the extent of lateral mixing
2. Mature cement, low mixing – high pH (about 12), moderate ionic strength, with key parameters dependent on the extent of lateral mixing
3. Mature cement, high mixing – circumneutral pH (about 7), moderate ionic strength, with key parameters dependent on the extent of lateral mixing
4. Degraded cement, low mixing – high pH (about 11), moderate ionic strength, with key parameters dependent on the extent of lateral mixing
5. Degraded cement, high mixing – circumneutral pH (about 7), moderate ionic strength, with key parameters dependent on the extent of lateral mixing.

The external surfaces of the vault system will be exposed to high infiltration rates during the 50-year operation period prior to closing the vault and emplacing the soil cap. This will likely wash all external surfaces and result in these surfaces behaving as mature cement. This external washing, in combination with the different flow regimes that will determine the solution composition of water infiltrating into the vault (e.g., transport through a network of cement cracks) and beneath the vault (e.g., transport across cement surfaces), suggest that water in the RH-LLW vault underlayment will most likely be interacting with either mature or degraded cement. Consequently, the fresh cement scenario can be discarded. For the mature and degraded cement, there are two clear scenarios. With low mixing, the solution chemistry in the RH-LLW vault underlayment is equivalent to water in equilibrium with mature cement. With high mixing, the solution chemistry is comparable to natural waters.

#### *3.5.1.1 Conceptual Approach for Evaluating the Impact of Cement Leachate on $K_d$ Values for Sediment Beneath the Remote-Handled Low-Level Waste Facility.*

Kaplan (2010) has developed a geochemical data package to estimate the $K_d$ for radionuclide transport in silts and sediment at the Savannah River Site by developing a "cement leachate impact factor," specific to individual radionuclides and that alters $K_d$ from what it would be under natural conditions to an alternate value that is more reflective of transport in cement-impacted solutions. Cement leachate impact factors greater than one are indicative of increased retention within soils (e.g., higher $K_d$), while factors less than one indicate reduced retention within soils (e.g., lower $K_d$). Kaplan's base $K_d$ values were experimentally measured on Savannah River Site sediment, while his cement leachate impact factors were largely derived from experiments conducted at Pacific Northwest National Laboratory to determine the potential impact of high pH, from leaking tanks, on radionuclide transport (Cantrell et al. 2007, Cantrell et al. 2008). The Pacific Northwest National Laboratory experiments evaluated the impact of caustic, high-salinity tank waste on radionuclide sorption to a range of sediment types.

Cement leachate impact factors provided in these previous analyses were not derived from experimental data using the cement, sand/gravels, or alluvium that will be deployed in the RH-LLW disposal facility. There are significant differences in liquid and vapor phase chemistry, soil mineralogy,

cement composition, temperature, radionuclide residence times, and overall water-refresh (infiltration) rates. These differences could cause the observations from the INL system to deviate from those measured by Kaplan and Cantrell in significant ways. Also, the impact factors provided by Cantrell and Kaplan exhibit a large range of variability – presumably related to differences in materials and conditions evaluated. In as much as the impact factors may not be representative of INL conditions, they are the only data available that provide guidance on how cement leachate could potentially alter the $K_d$ values for radionuclide transport through both the RH-LLW underlayment and the underlying alluvium. In the absence of data that are directly applicable to INL, these impact factors provide the best estimate that can be made on the basis of literature reports. This report adopts these factors only after considering them in light of established knowledge of the behavior of the key radionuclides in environments where pH and ionic strength are elevated through reactions between dissolving minerals (e.g., cement) and infiltrating groundwater of a known composition (e.g., INL alluvium water). These impact factors are approximate and the values have not been verified with confirmatory analyses. However, they are consistent with standard geochemical theory and do provide useful insight for these bounding calculations.

The cement leachate impact factors reported by Kaplan (2010) are reported in Table 16, as are alternate factors calculated by applying the same approach to different datasets. In interpreting data and calculations provided in Table 16, it is important to note that the calculations reported by Kaplan (2010) contain confusing data references. The authors have conferred with Kaplan and discovered that Cantrell et al. (2007) altered what data tables they present and where during final revisions. The references in Kaplan (2010) refer to data in earlier versions of Cantrell et al. (2007) and not as the report was finally published. Specifically, the data for "IDF cementitious waste" that Kaplan (2010) refers to as Table 3.2 and Table 3.10 of Cantrell et al. (2007) is actually located in Table B.1 (page B.4) of Cantrell et al. (2007). The table that Kaplan (2010) refers to as listing "Hanford best groundwater $K_d$" seems to have been omitted, with the text of Cantrell et al. (2007) actually listing general $K_d$ ranges and referring to the Hanford $K_d$ database (Cantrell et al. 2003). Kaplan (2010) used these two sets of values to calculate the cement leachate impact factors in his report. These values, as well as the basis for the recommendations given in Kaplan (2010), are provided in columns 2 through 4 of Table 16.

Close inspection of the $K_d$ data reported in the relevant Hanford groundwater reports (Cantrell et al. 2003, Cantrell et al., 2007, Cantrell et al., 2008) reveal discrepancies between datasets provided in these reports that do not have a clear explanation. There is not a clear set of comprehensive analyses of Hanford groundwater that can lead to a rigorous conclusion regarding how cement leachate impacts radionuclide sorption; and, subsequently, how cement leachate solutions could impact $K_d$ values in INL sands and alluvium sediment. This report addresses this issue by applying the approach of Kaplan (2010) to these different datasets and deriving a range values for cement leachate factors. These values are provided in columns 5 through 10 of Table 16. The cement leachate factor recommended for use in the sediment underlying the RH-LLW facility and the basis for this recommendation are given in columns 11 through 12 of Table 16.

Recommended cement leachate impact factors are also provided in Table 16. This report generally recommends the lowest cement leachate impact factor that can be derived from the Pacific Northwest National Laboratory data (Cantrell et al. 2007, Cantrell et al. 2008) and the geochemical interpretations provided by Kaplan (2010). For U, Ni, Np, and Pb, the different reports suggest a wide range of potential cement leachate impact factors and an intermediate value is recommended. For uranium, Cantrell et al. (2007) report that glass-waste leachates at Pacific Northwest National Laboratory do not contain sufficient $Ca^{2+}$ to scavenge carbonate anions that lower uranium $K_d$. We anticipate $Ca^{2+}$ to be present in the INL system and have selected the lowest estimated cement leachate impact factor that is not specific to unique glass-leachate waste conditions reported by Cantrell et al. (2007). For Ni, Np, and Pb, there is no consistent trend that can describe the range in reported ratios between $K_d$ for impacted and unimpacted sediment. Cantrell et al. (2007 and 2008) do not provide detailed analysis of the discrepancies. The only conclusion possible at this time is that the range arises from undefined site-specific factors that are not

likely to be operable at the INL Site. In the absence of reports that allow some contrast with INL conditions, this analysis recommends the cement leachate impact factor value that is intermediate between all information resources provided in Table 16.

#### *3.5.1.2 Application of the Conceptual Approach to Estimating $K_d$ Values for Sediment Beneath the Remote-Handled Low-Level Waste Facility.*

The absence of site-specific data relevant to a cement-impacted environment at the RH-LLW facility does not eliminate the need to estimate conservative $K_d$ values for radionuclide sorption in a cement-impacted alluvium environment. To address this problem, this report uses data from multiple measurements made in the unique environment at Pacific Northwest National Laboratory in order to estimate potential values for alkaline leachate impact factors. These estimates of potential "cement leachate impact factors" are then applied to $K_d$ estimates for native INL alluvium to estimate $K_d$ values for cement-impacted INL alluvium. This is the most reasonable approach that can be employed in the absence of confirmatory analyses.

## 3.6 Distribution Coefficient Values for Sand/Gravel Underlayment and Alluvium Sediment Impacted by Cement Leachate

In the absence of site-specific data under anticipated in situ conditions, this report recommends that the impact of cement leaching on contaminant sorption onto INL sediment be estimated using the cement leachate impact factor method developed by Kaplan (2010). According to Equation 7

$$K_d \text{ (cement-impacted)} = K_d \text{ (natural conditions)} * \text{cement leachate impact factor} \quad (7)$$

Estimated $K_d$ values for natural conditions are given in Table 14 for sand and Table 15 for RH-LLW alluvium. Estimated cement leachate impact factors are provided in Table 16. Based on these data, estimated $K_d$ values for cement-impacted sand/gravel underlayment are provided in Table 17, using Equation 7. $K_d$ values for cement-impacted alluvium, using Equation 7, are provided in Table 18.

## 3.7 Impact of Cellulose Degradation Products on Distribution Coefficient Values for the Sand/Gravel Underlayment and Alluvium Sediment

Kaplan (2006, 2010) reports that the degradation products from cellulosic materials (e.g., wood, paper, and cardboard) can impact contaminant transport. The impacts of CDP are dependent on numerous factors, including sediment chemistry, radionuclide geochemistry, and the mass concentration of organic complexing agents. At low concentration, CDP can increase radionuclide sorption and retard transport. At high concentration, CDP can lower $K_d$ and enhance radionuclide transport. Also, CDP constituents are subject to biodegradation and are likely to have environmental half-lives much lower than the radionuclides they interact with. Their impact is likely to be transitory. This transitory nature of CDP impacts is important to consider because the cement floor of the RH-LLW vault is likely to bind most radionuclides very strongly (e.g., Table 13). Consequently, it is likely that organic matter will be transported out of the vault and alluvium and degraded before the radionuclides they may impact even pass beyond the cement floor. Even if there is some interaction, the different timing of radionuclide and CDP pulses is likely to place CDP concentrations at lower levels than Kaplan (2006, 2010) reports to increase the sorption of most radionuclides. Given all of the competing factors involving the mass concentration of CDP and the different timing of CDP and radionuclide transport out of the vault and into the alluvium, it is likely that the impact of CDP on radionuclide sorption will be negligible. Despite these considerations, it is important to document the bounding scenarios for all factors that could potentially impact $K_d$ values in a significant way. This study adopts the approach of Kaplan (2006, 2010) and provides estimated CDP impact factors for radionuclide $K_d$. These impact factors modify $K_d$ as follows:

$$K_d \text{ (CDP-impacted)} = K_d \text{ (absence of CDP)} * \text{CDP impact factor} \quad (8)$$

Table 16. Derivation of potential cement leachate impact factors for distribution coefficient estimates in Idaho National Laboratory alluvium and sand/gravel sediment in the vault underlayment. Data from measurements by Cantrell et al. (2007 and 2008) on sandy sediment at the Pacific Northwest National Laboratory. Derivation of cement leachate impact factor as per Kaplan (2010). The estimated distribution coefficient for radionuclide sorption to sediment impacted by caustic cement leachate is the product of a distribution coefficient measured under natural conditions and the cement leachate impact factor reported herein.

| | Cement Leachate Impact Factors for Hanford IDF Cementitious Waste (Kaplan 2010) | | | Alternate Calculation from Experimental Data reported in Appendix C of Cantrell et al. (2007) | | | Alternate Calculation Cement Leachate Impact Factor from Experimental Data reported in Table 3.4 and Table 3.9 of Cantrell et al. (2008) | | | Cement Leachate Impact Factors Recommended for RH-LLW Underlayment and Alluvium | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Radionuclide | As Kaplan calculates from PNNL data (Cantrell et al. 2007) | As recommended in Table 2, 22 of Kaplan (2010) | Basis for Kaplan Recommendation for Cement Leachate Impact Factors (Kaplan 2010) | Best $K_d$ for Nonimpacted Far Field in Sand Sequence (Table C.6) | Best $K_d$ for Chemically Impacted Far Field Sand Sequence (Table C.5) | Cement Leachate Impact Factor Derived per (Kaplan 2010) | Sand-Sized Sediment, Best $K_d$ Estimate, No Waste Impact (Table 3.4) | Sand-Sized Sediment, Best Intermediate Impact, Waste Areas A,C (Table 3.3, 3.9) | Cement Leachate Impact Factor. Derived per (Kaplan 2010) | Cement Leachate Impact Factor (unitless) | Basis |
| Ac-227 | — | 1.5 | Similar chemistry to Eu | 300 | 350 | 1.2 | — | — | — | 1.2 | Conservative, comparable to Kaplan (2010) |
| C-14 | — | 5 | None given | 5 | 20 | 4 | 5 | 1 | 0.2 | 4 | Conservative, comparable to Kaplan (2010) |
| Cl-36 | — | 0.1 | Similar chemistry to Tc | 0 | 0 | 1 | — | — | — | 0.1 | Conservative, per Kaplan (2010) |
| H-3 | — | 1 | None given | 0 | 0 | 1 | 0 | 0 | 1.0 | 1 | Per Kaplan (2010) |
| I-129 | 1 | 0.1 | Separate experiments by Kaplan with PNNL sediment | 0.25 | 0.1 | 0.4 | 0.2 | 0.2 | 1.0 | 0.1 | Conservative, comparable to Kaplan (2010) |
| Mo-93 | — | 1.4 | Anion chemistry similar to Se | — | — | — | — | — | — | 1.4 | Per Kaplan (2010) |
| Nb-94 | — | 1.4 | Anion chemistry similar to Se | — | — | — | — | — | — | 1.4 | Per Kaplan (2010) |
| Ni-59 | — | 3.2 | Half the impact factor observed for Sr in PNNL experiments | 300 | 80 | 0.3 | 300 | 3 | 0.01 | 0.3 | See text |
| Np-237 | 1.5 | 1.5 | — | 15 | 0.8 | 0.1 | 10 | 10 | 1.0 | 1 | See text |
| Pb-210 | — | 3.2 | Half the impact factor observed for Sr in PNNL experiments | 10,000 | 100 | 0.01 | 50 | 10 | 0.2 | 0.2 | See text |
| Plutonium (multiple) | — | 2 | Pu is solubility controlled, did not consider colloids | 150 | 200 | 1.3 | 600 | 600 | 1.0 | 1.3 | Conservative, comparable to Kaplan (2010) |
| Protactinium (multiple) | — | 1.5 | Similar chemistry to Np | — | — | — | — | — | — | 1.5 | Per Kaplan (2010) |
| Radium (multiple) | — | 3 | Equivalent to Sr | 14 | 10 | 0.7 | 20 | 10 | 0.5 | 0.5 | Conservative, lowest of recalculated values |
| Sr-90 | 6.4 | 3 | Basis is unclear | 14 | 10 | 0.7 | 20 | 10 | 0.5 | 0.5 | Conservative, lowest of recalculated values |
| Tc-99 | — | 0.1 | High pH will reduce anion exchange | 0 | 0 | 1 | 0 | 0.1 | NA | 0.1 | Per Kaplan (2010) |
| Thorium (multiple) | — | 2 | Basis is unclear | 1,000 | 300 | 0.3 | — | — | — | 0.3 | Conservative, lowest of recalculated values |
| Uranium (multiple) | 1.25 | 5 | Kaplan anticipates uranyl precipitation | 1 | 0.2 | 0.2 | 0.8 | 0.8 to 2 | 1 to 2.5 | 1 | See text |

Note that the CDP impact factor should be considered in addition to the cement leachate impact factor. If both CDP and cement-leachate are thought to be present, then the combined impact is equal to the product of the "natural condition" $K_d$ and both the cement-leachate and CDP impact factors. Estimated $K_d$ values for natural conditions are given in Table 14 for sand and Table 15 for RH-LLW alluvium. Estimated CDP impact factors are provided in Table 19 as a function of the concentration of aqueous organic carbon. For all cases, except Ac-227, the estimated most likely CDP impact factor is greater than or equal to 1, suggesting that CDP will enhance sorption or have no significant impact. In order to provide the most robust bounding scenarios, this study recommends a CDP impact factor of 1 for all elements except, Ac-227 (e.g., negligible CDP impact). For Ac-227, a value of 0.8 is recommended.

## 3.8 Distribution Coefficient Values for Interbed Sediment

Based on available mineralogy, grain size, CEC, and solution chemistry, minimum $K_d$ values for alluvium and interbed sediment should be comparable. Given the aspect ratio of the RH-LLW disposal facility and depth to the interbeds, it is likely that infiltration from areas adjacent to and beneath the facility mixes with water not encountering the vault system. As a result, the mixing that occurs at depth suggests cement impacts anticipated for the RH-LLW alluvium will not occur in the interbed sediment. It also is likely that this mixing will reduce the concentration of cellulose degradation products to levels below which they measurably impact contaminant sorption. In the absence of site-specific measurements, it is recommended that native water $K_d$ values for alluvium also be used for interbed sediment. These values are given in Column 5 of Table 18.

## 3.9 Distribution Coefficient Values for Basalt

This analysis assumes that basalt has negligible reactivity; therefore, $K_d$ is equal to 0 mL/g for all contaminants. This is conservative because all contaminants will interact with the basalt and infill sediment surfaces to a limited extent and will have a $K_d$ value greater than zero. The other reactive zones are anticipated to have significantly greater $K_d$ values.

# 4. SUMMARY OF KEY GEOCHEMICAL CONSIDERATIONS

The RH-LLW vault is a complex and dynamic system that introduces many artificial constituents that have the potential to alter the system's geochemical and transport properties in ways that are not well understood. In some cases and for some radionuclides, the alterations are likely to reduce transport rates and concentrations once the radionuclides escape the waste container. In others cases, the alterations could be detrimental. This report provides an initial assessment of the range of conditions expected. To reduce uncertainty in predicted system performance, the following information would be useful:

- Solution chemistry of typical INL alluvium water that has migrated through cement pores and slowly transported across cement surfaces.
- Solution chemistry of INL alluvium water that is in contact with sand and cement surfaces under spatial and hydraulic conditions emulative of the vault system.
- Measurements of steel corrosion and corrosion impacts on solution chemistry under vault conditions.
- Measurements of steel and metal corrosion inside waste containers under vault conditions and the impact of that corrosion on solution chemistry.
- Chemistry of interactions between radionuclides and cement-impacted water.
- Chemistry of interaction between radionuclides and INL alluvium sediment under the wide range of solution conditions that could occur in the alluvium beneath the RH-LLW vault.
- Coupling or feedbacks between the different components of the system that may impact overall system performance.

The objective of this report is to provide $K_d$ estimates to support the performance assessment of a low-level nuclear waste disposal facility at INL. This objective has been met through an assessment of potential geochemical conditions existing throughout the lifetime of the facility and of their impacts on the overall cement, metal, soil, and water environment. In addition to heterogeneous material properties, the long timeframes involved introduce uncertainty in the most likely Kd values. The range of uncertainty has been bounded through an assessment of most likely minimum and most likely maximum $K_d$s. The range of values provided allows for adequate assessment of mean facility performance while providing the basis for uncertainty analysis.

The information provided here should be sufficient for probabilistic performance assessment calculations. Uncertainty could be reduced through collection and evaluation of site-specific sediment properties, pore-water chemistry, and cement compositions in combination with geochemical transformation modeling over the life cycle of the facility.

Table 17. Estimated distribution coefficient values (mL/g) for sand/gravel underlayment under native alluvium water and cement-impacted groundwater conditions.

| Radionuclide | Sand, Most Likely Minimum ($K_d$, mL/g) | Sand, Most Likely Actual ($K_d$, mL/g) | Sand, Most Likely Maximum ($K_d$, mL/g) | Natural Sand, Recommended ($K_d$, mL/g) | Cement Leachate Impact Factor | Cement Impacted Sand, Recommended ($K_d$, mL/g) |
|---|---|---|---|---|---|---|
| Ac-227 | 60 | 300 | 1,100 | 60 | 1.2 | 72 |
| C-14 | 0 | 5 | 10 | 0 | 4 | 0 |
| Cl-36 | 0 | 0 | 0 | 0 | 0.1 | 0 |
| H-3 | 0 | 0 | 0 | 0 | 1 | 0 |
| I-129 | 0 | 0 | 0.3 | 0 | 0.1 | 0 |
| Mo-93 | 0 | 1 | 1,000 | 1 | 1.4 | 1.4 |
| Nb-94 | — | — | — | 0 | 1.4 | 0 |
| Ni-59 | 7 | 50 | 300 | 7 | 0.3 | 2.1 |
| Np-237 | 2 | -- | 15 | 2 | 1 | 2 |
| Pb-210 | 10 | 2,000 | 10,000 | 10 | 0.2 | 2 |
| Plutonium (multiple) | 10 | 50 | 200 | 16 | 1.3 | 21 |
| Protactinium (multiple) | — | 3 | — | 3 | 1.5 | 4.5 |
| Radium (multiple) | — | 5 | 14 | 5 | 0.5 | 2.5 |
| Sr-90 | 5 | 10 | 14 | 5 | 0.5 | 2.5 |
| Tc-99 | 0 | 0 | 0 | 0 | 0.1 | 0 |
| Thorium (multiple) | — | 40 | 1,000 | 40 | 0.3 | 12 |
| Uranium (multiple) | — | 0.2 | 1 | 0.2 | 1 | 0.2 |

Table 18. Estimated distribution coefficient values (mL/g) for remote-handled low-level waste alluvium under native alluvium water and cement-impacted groundwater conditions.

| Radionuclide | Alluvium, Most Likely Minimum ($K_d$, mL/g) | Alluvium, Most Likely Actual ($K_d$, mL/g) | Alluvium, Most Likely Maximum ($K_d$, mL/g) | Natural Alluvium, Recommended ($K_d$, mL/g) | Cement Leachate Impact Factor | Cement Impacted Alluvium, Recommended ($K_d$, mL/g) |
|---|---|---|---|---|---|---|
| Ac-227 | 225 | 300 | 1,500 | 300 | 1.2 | 360 |
| C-14 | 0 | 0.5 | 2.4 | 0.5 | 4 | 2 |
| Cl-36 | 0 | 0 | 0 | 0 | 0.1 | 0 |
| H-3 | 0 | — | 0.1 | 0 | 1 | 0 |
| I-129 | 0 | 2.8 to 7 | 8.7 | 3 to 7 | 0.1 | 0.3 to 0.7 |
| Mo-93 | 10 | — | 125 | 10 | 1.4 | 14 |
| Nb-94 | 160 | — | 550 | 160 | 1.4 | 224 |
| Ni-59 | 100 | — | 400 | 100 | 0.3 | 30 |
| Np-237 | 11 | 17.5 | 24 | 18 | 1 | 18 |
| Pb-210 | 100 | 270 | 16,000 | 270 | 0.2 | 54 |
| Plutonium (multiple) | 280 | 1,140 | 2,680 | 1,140 | 1.3 | 1,480 |
| Protactinium (multiple) | 8 | 550 | 1,800 | 550 | 1.5 | 825 |
| Radium (multiple) | 100 | 500 | 36,000 | 500 | 0.5 | 250 |
| Sr-90 | 5 | 22 | 39 | 22 | 0.5 | 11 |
| Tc-99 | 0 | 0.1 | 1.4 | 0.1 | 0.1 | 0 |
| Thorium (multiple) | 100 | 500 | 3,300 | 500 | 0.3 | 150 |
| Uranium (multiple) | 6 | 10 | 11 | 10 | 1 | 10 |

Table 19. Estimated cellulose degradation product impact factors for target radionuclides at various levels of organic matter loading (values adopted from Kaplan (2006, 2010).

| Radionuclide | Kaplan (2006) (10 mg/L C) | Kaplan (2006) (20 mg/L C) | Kaplan (2006) (95 mg/L C) | Kaplan (2006) (222 mg/L C) | Kaplan (2010), concentration not given | Most Likely CDP impact factor |
|---|---|---|---|---|---|---|
| Ac-227 | 2.9 | 0.77 | 0.049 | 0.015 | 0.55 | 0.8 |
| C-14 | — | — | — | — | 1 | 1 |
| Cl-36 | — | — | — | — | 1 | 1 |
| H-3 | — | — | — | — | 1 | 1 |
| I-129 | — | — | — | — | 1 | 1 |
| Mo-93 | — | — | — | — | 1 | 1 |
| Nb-94 | — | — | — | — | 1 | 1 |
| Ni-59 | 1.13 | 1.82 | 1.41 | 0.88 | 1 | 1.8 |
| Np-237 | 1.14 | 1.14 | 1.66 | 1.49 | 1 | 1.1 |
| Pb-210 | 1.13 | 1.82 | 1.41 | 0.88 | 1 | 1.8 |
| Plutonium (multiple) | 1.89 | 2.92 | 0.51 | 0.12 | 1 | 2.9 |
| Protactinium (multiple) | — | — | — | — | 1 | 1 |
| Radium (multiple) | — | — | — | — | 1 | 1 |
| Sr-90 | 1.22 | 2.38 | 1.89 | 0.44 | 1 | 2.4 |
| Tc-99 | — | — | — | — | 1 | |
| Thorium (multiple) | 1.89 | 2.92 | 0.51 | 0.12 | 1 | 2.9 |
| Uranium (multiple) | 1.22 | 2.38 | 1.89 | 0.44 | 1 | 2.4 |

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# Appendix A

# Documentation of Geochemical Model for Evaluation of factors that Impact Contaminant Sorption at the Remote-Handled Low-Level Waste Facility

This appendix provides supporting information that describes how geochemical modeling was used to estimate how emplacement of a cement vault in INL alluvium sediment would impact solution chemistry in multiple zones within the vault interior and in the underlying sediment. This model was constructed within PHREEQC (version 2.17.5), which is a geochemical modeling program developed by the United States Geological Survey and commonly used for geochemical simulations and analyses. This appendix describes the modeling approach used, the assumptions made, data inputs, and sample results. It also provides a validation of model calculations. This presentation assumes that the reader is familiar with PHREEQc and is experienced in the application of this modeling code to geochemical calculations.

## A-1. MODELING APPROACH

All geochemical modeling calculations were conducted with PHREEQC, which is an established geochemical modeling code with a large user community and experience base. As stated on the United States Geological Survey's website (http://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqc/), PHREEQC version 2 is a computer program written in the C programming language that is designed to perform a wide variety of low-temperature aqueous geochemical calculations. PHREEQC is based on an ion-association aqueous model and has capabilities for (1) speciation and saturation-index calculations; (2) batch-reaction and one-dimensional transport calculations involving reversible reactions, which include aqueous, mineral, gas, solid-solution, surface-complexation, and ion-exchange equilibria, and irreversible reactions, which include specified mole transfers of reactants, kinetically controlled reactions, mixing of solutions, and temperature changes; and (3) inverse modeling, which finds sets of mineral and gas mole transfers that account for differences in composition between waters, within specified compositional uncertainty limits. PHREEQC also can simulate dispersion (or diffusion) and stagnant zones in one-dimensional-transport calculations, model kinetic reactions with user-defined rate expressions, model the formation or dissolution of ideal, multicomponent or nonideal, binary solid solutions, model fixed-volume gas phases in addition to fixed-pressure gas phases, allow the number of surface or exchange sites to vary with the dissolution or precipitation of minerals or kinetic reactants, include isotope mole balances in inverse modeling calculations, and automatically use multiple sets of convergence parameters. When teamed with the PHAST groundwater flow model, these programs can also simulate multicomponent, reactive solute transport in three-dimensional saturated groundwater flow systems. These simulation programs have a large user-community and are maintained and updated by the United States Geological Survey.

## A-2. BASIS FOR USING BATCH MODE CALCULATIONS

PHREEQC can conduct batch calculations, one-dimensional transport calculations, and one-dimensional transport calculations plus diffusion. When combined with PHAST, the two models can also conduct multi-dimensional reactive transport calculations using a range of hydrologic and geochemical approaches. However, this project utilized batch-mode geochemical calculations. This decision was made for the following reasons:

- The project was operating under tight time constraints and batch calculations are much simpler to parameterize, solve, and interpret than transport calculations.

- The system is exceedingly complex and it is not clear that the extra effort required to conduct reactive transport calculations would provide commensurate added value. The calculations can be done, but further assumptions would be needed and more detailed calculations would not necessarily be more meaningful.
- The purpose of the modeling exercise was not to predict sorption of radionuclide contaminants, but rather to estimate a range of potential future geochemical scenarios so that appropriate conservative $K_d$ values could be extrapolated from the literature.
- Reactive transport calculations, based in part on the $K_d$ recommendations, were being conducted by another team, with a computer code designed to predict risk of multi-pathway exposure to radionuclide contaminants. Additional transport calculations may have been duplicative or ancillary to the primary objective of this task.

Based on these considerations, the modeling approach in PHREEQC needed to provide information that could be used to bound potential scenarios to be assessed in risk calculations. The objective was *not* to discover the most likely geochemical scenario; but rather to discover what is "the best" or "the worst" that could reasonably be expected to occur. Modeling efforts need to support the estimation of conservative $K_d$ values for a large number of radionuclides where (1) few measured values relevant to INL sediment under "native" conditions were available and (2) no data on radionuclide sorption to INL sediment under cement-impacted conditions was available. Consequently, there is scarce data available to validate model calculations. This lack of data substantially limits the ability of geochemical models to predict impacts that might occur far into the unknown future. Initial conditions are not well characterized and key processes that may impact future events have not been evaluated in a site-specific way. Given these limits to current knowledge, modeling efforts were designed to answer a narrow set of questions:

1. How could interaction with cement surfaces and iron rebar in cracks and pores within the vault ceiling alter the composition of influent native alluvium water?
2. How could corrosion of steel drums (liners) alter the chemistry of infiltrating alluvium water that has previously reacted with cement and rebar?
3. How could corrosion of metal reactor parts within the liners further alter solution composition?
4. What is a reasonable range of potential values for pH, oxidation state, and major ions for solutions in contact with waste anion-exchange resins, corroding steel reactor parts, and combinations of the two?
5. What is reasonable range of potential values for pH, oxidation state, and major ions for solution in contact with aged cement surfaces at the bottom of the cement vault?
6. How could solution composition in the alluvium beneath the vault change under different mixing scenarios between water that has equilibrated with aged surfaces of cement and native alluvium water that has infiltrated through alluvium backfill?

These questions were investigated through batch-mode calculations using the PHREEQc modeling code. For each level of the system, the composition of "upstream" components was used as a model input to define the composition of "downstream" components. In this way, calculations proceeded downward from the cap to the interbeds and aquifer (e.g. Figure 1). At each level, simplifying assumptions were made. Each of these assumptions was intended to reflect the likely maximum negative impact of the vault system on radionuclide transport through the underlying sediment. In this way, we progressively defined the system to reflect maximum likely radionuclide transport and calculated the range of solution composition accordingly. The solution composition was then used as a guide for estimating which $K_d$ values from the literature to recommend for use in reactive transport modeling.

# A-3. STRUCTURE OF BATCH MODE CALCULATIONS

For the purposes of "sequential batch" modeling, the hydrogeochemical system was considered to consist of different components. Each of these components has different hydrological and geochemical properties and provides forcing factors that impact the systems' geochemical properties and the resultant range of potential $K_d$ values. System components are as follows:

- *Infiltrating water* – Provides chemical constituents that act in concert with soil and waste repository surfaces to determine solution chemistry and provides a medium for contaminant transport.
- *Soil cap (alluvium)* – Controls the rate of infiltration and reacts with infiltrating rain and snow water, increasing ionic strength and buffering the pH of precipitation-derived water. It is assumed to consist primarily of native alluvial sediment. Alluvium also will bound the lateral extent of the facility.
- *Repository vault* – Isolates the waste containers from infiltrating water and reduces the extent of geochemical interaction between waste and water. The vault is constructed of cement and iron rebar, which will react with water to elevate ionic strength and buffer pH to a level more basic than would occur in a soil-water system. Cement also provides a surface for radionuclides to adsorb onto.
- *Steel waste containers (liners)* – Isolates the waste from infiltrating water and reduces the extent of geochemical interaction between waste and water. Steel liners will corrode in the presence of water, altering pH, oxidation state, and solution composition as they degrade.
- *Waste* – Provides the radionuclides being transported.
- *RH-LLW vault underlayment (sand/gravel base)* – Improves the structural integrity of the vault. Underlayment is assumed to consist of sand and gravel and can alter solution chemistry through sorption and mineral dissolution/precipitation reactions.
- *Native alluvium soil* – This is native sediment that underlies the vault and the sand and gravel base. It extends from the bottom of the vault underlayment to the top of the basalt. It is anticipated to have the same mineralogical composition as the alluvium cap material. It provides surfaces for radionuclides to adsorb onto and may alter solution geochemistry.

Each of these components sequentially impacts the composition of the layer beneath it (Figure 1). Therefore, any effort to understand how the vault will impact the sorption of contaminants in the underlying alluvium and interbeds must begin at the cap and trace water downward. The modeling approach does this by using PHREEQC to conduct simplified, "first-order" bounding calculations. Each component of the system was modeled individually via a batch calculation. The different batch calculations were linked so that the output of one contributed to the input of another. This approach excludes key elements of the system such as layered degradation of cement surfaces coupled to diffusive transport from cement pores to cement surfaces exposed by cement cracks. As such, the modeling approach is not comprehensive and only provides a first-order approximation.

## A-3.1 Hydrogeochemical Assumptions

The "sequential batch" mode calculations must account for both initial conditions and time-variable processes that can modify the system's hydrogeochemical conditions. The structure and outcome of the calculations depends strongly on the assumptions used. Thus, to understand the basis for the calculations described herein, it is important to clearly state these assumptions. The assumptions applicable to each of the components outlined above, as well as for initial conditions, are enumerated in the following sections.

# A-4. INITIAL CONDITIONS

During the first 50 years, radioactive waste will be deposited in steel liners emplaced into concrete vaults at the RH-LLW facility. The facility will be actively maintained while waste accumulates. Snow will be removed and rainwater managed to reduce contact with the waste containers. Water that does

enter the facility will come in contact with the cement walls of the repository, and contact with the waste liners will be kept to a minimum. These operational parameters provide the basis for the assumptions that establish the initial conditions of the vault's outer surfaces and state of the waste and waste containers.

- The waste containers will not corrode significantly within the first 50 years.
- There will be no important geochemical reactions within the waste containers over the first 50 years.
- The surfaces of the cement in the vault will come into contact with water and will degrade from fresh cement state to either mature cement or degraded cement.

## A-5. Infiltrating Water and Soil Cap

After 50 years, an engineered cover (cap) will be placed over the RH-LLW repository. At this point, water infiltrating into the RH-LLW facility will need to pass through the cap before reaching the vault. This operation parameter provides the basis for assumptions that describe the initial conditions for water that penetrates into the vault.

- The engineered barrier (alluvium cap) will be composed of fine-grained surficial sediment gathered from an uncontaminated location at the INL site.
- Soil water in the cap will have a composition similar to that of uncontaminated INL alluvium sediment.
- Data gathered from analysis of alluvium water in uncontaminated regions of INL provide a good proxy for soil water that will come in contact with the vault.

## A-6. Repository Vault

Water can enter the repository vault in one of two ways: (1) enter the vault as soil moisture and condense on cement or steel surfaces or (2) infiltrate through the cap, pool at the top of the vault, and slowly penetrate into the vault through cement pores and cracks that form in the cement. In either case, water will react with cement. Depending on residence time in contact with the cement and extent of prior reactions, these reactions will increase pH, increase ionic strength, and change the major ion content of the solutions inside the repository vault. In the case of gaseous soil moisture, deionized water will be in contact with cement surfaces. In the case of infiltrating water, the composition of the influent solution is as described previously. *The model assumes that the majority of water entering the vault will have infiltrated through the soil cap and subsequently through cracks and pores in the cement.*

The composition of the solution that enters the vault and corrodes the steal liners depends on two factors: (1) the composition of the influent solution and (2) geochemical reactions between cement and infiltrating water. Model calculations involving the reaction of influent water with cement are founded upon the following assumptions:

- All pore volume in concrete is filled with water.
- The entire mass of concrete per liter of pore volume of the porous concrete medium is able to come to equilibrium with solution.
- The cement to be used is a Hydrated Sulphate-Resistant Portland Cement with a mineral composition as specified in Table 5.
- In addition to the assumed native porosity of cement (Table 5), the cement will have 10% additional porosity due to crack formation. These cracks will be hydraulically connected to the cement pores.
- The concrete will contain iron rebar, with a composition that is 98% Fe and less than 2% other metals (C, Mn, P, S, Cr, Cu, Ni, Mn, and Mo). The rebar constitutes 12.5% by mass of total reinforced concrete.

- The iron rebar will corrode at a rate comparable to that of carbon steel at near neutral pH. This rate can be estimated from the data of Adler-Flitton (2004).

These assumptions will simulate a system that is technically inaccurate in several regards. First, the assumption that the entire mass of concrete is able to react with infiltrating solution overstates the extent of cement degradation that will likely occur. In reality, only the surfaces of cracks are likely to be exposed to water. Those will rapidly degrade and access to the fresh cement that constitutes most of the mass will be limited by diffusion. Therefore, after an initial period, the water in the pores is more likely to reflect interaction with mature or degraded cement than interaction with fresh cement. Second, the actual composition of the cement used is likely to be somewhat different from the assumed composition; which is based on published papers rather than technical specifications for the project. Third, the mass and composition of iron rebar is likely to be different than assumed. Fourth, the steel in rebar will likely corrode much more slowly than assumed because elevated pH inhibits corrosion. Finally, the crack density and crack porosity will likely be different than is assumed.

The PHREEQc model assumes saturated flow through cement with 10% additional porosity due to cracking. This yields a total porosity of 31% if it is further assumed that native porosity and cracks are hydraulically connected. Cement properties are otherwise as described in Column 3 of Table 6, with the further assumption that reinforced concrete contains 12.5% carbon steel by mass and 87.5% by mass Hydrated Sulphate-Resistant Portland cement. At 31% porosity, there is

- 3.2 $m^3$ of reinforced concrete per cubic meter aqueous solution.
  - Reinforced concrete has a density of approximately 2,400 kg per $m^3$
  - Each cubic meter of porous reinforced concrete contains 2,090 kg cement, 310 kg of steel rebar, and 312 kg of water (density = 1000 kg / cubic meter)
- This equates to approximately 6.7 kg cement per kg water and 1 kg steel per kg water.

The geochemical model is calculated on the basis of kilograms aqueous solution. Thus, each kg of infiltrating water is assumed to react with 1 kg of steel rebar and 6.7 kg of cement (e.g. 6.7 * values in column 3 of Table 1). Three different types of cement compositions were considered: fresh, mature, and degraded. The selection of cement type does not change the theoretical basis of the model, it only changes the mineral composition of the cement. Fresh cement is as described in Table 5. Mature cement is assumed to be as described in Table 5, excluding KOH and NaOH (soluble hydroxides washed out). Degraded cement is defined as cement where solution pH is controlled by a mixture of calcite and CSH gel with a minimum Ca/Si ratio. The composition of degraded cement is assumed to be equivalent to a system where all portlandite is replaced with calcite and 25% of all CSH gel is replaced by a mixture of amorphous silica ($SiO_2$-am) and calcite. All remaining CSH gel has a Ca/Si ratio of 0.25.

## A-7. Steel Waste Liners

Steel waste liners will begin to corrode on external surfaces when infiltrating water encounters them. They will begin to corrode on internal surfaces once any anti-corrosive coatings have been compromised. Steel corrosion will further alter solution chemistry, reducing pH and potentially changing major ion content through a combination of aqueous-phase and precipitation reactions. The influent solution for this step is the effluent solution from the top of the cement vault. Model calculations involving the reaction of this influent water with steel are founded upon the following assumptions:

- Waste containers will consist of carbon steel. However, it is useful to conduct equivalent calculations for waste containers made of stainless steel.
- Carbon steel and stainless steel will corrode at a rate comparable to carbon steel and stainless steel coupons buried in INL sediment at near neutral pH. This rate can be estimated from the data of Adler-Flitton (INEEL/EXT-04-02335).

- Iron oxide passivation layers will not form and corrosion will continue uniformaly at a linear ($0^{th}$ order) rate.
- All water that enters the vault will react with waste liners. All water will move through the vault at a constant rate, which is the median of the anticipated number of pore volumes to move through the vault during the performance period.
- The moisture content of the vault will be assumed to be 10%, which is comparable to that of native INL alluvium.
- The gas composition in the vault will be the same as typical INL alluvium sediment.
- Infiltrating groundwater will not contain enough chloride to enhance steel corrosion
- The total mass of steel per unit volume can be estimated from preliminary data for NRF portion of the vault. Other contributors will have similar ratios of steel mass per unit volume.

These assumptions will simulate a system that is technically inaccurate in several regards. First, the corrosion data was measured at near-neutral pH while the liners will actually be exposed to water that has an elevated pH. Steel corrodes more slowly at high pH (e.g., references in $K_d$ report); therefore, actual corrosion will be less than assumed. Second, the actual amount of water to enter the system will likely be different and not all water entering the vault will encounter the waste liners. Third, the amount of water moving through the vault will vary over time, with slower initial infiltration rates transitioning to faster infiltration rates in later years. This could alter the results of calculations that are based on reaction kinetics. Fourth, once liners begin to corrode, iron oxide passivation layers will form and corrosion kinetics will be described by higher order equations.

As before, a simplified batch-mode model programmed into PHREEQc is used to conduct all geochemical calculations. Charge balance is not forced, but model performance is monitored to try and ensure that charge balance errors are less than 10%. System boundaries were established as follows:

- *Mass of steel* — Approximately 573,864 kg of carbon steel will be placed in 240,000 $ft^3$ of storage space at the NRF section of the RH-LLW facility. This equates to an effective steel density of approximately 85.4 kg steel per $m^3$ of vault space or approximately 1.0 to 1.5 moles iron per liter vault space.
- *Mineral phases* — Solution that has left contact with concrete and is now in contact with steel liners is assumed to exist in a simplified mineral system that consists of calcite, goethite, amorphous iron hydroxide, portlandite, and amorphous $SiO_2$.
- *Corrosion rate (Adler-Flitton et al. 2004)* — Mass loss from 19-$in.^2$ coupons buried in INL alluvium, with an average initial mass of 130 g over a 6-year experimental period.
  - From carbon steel, 10.5 ± 5.75 mmol iron per year. This equates to a mass loss of 80.8 ± 42.8 mmol iron lost per kilogram of carbon steel per year.
  - From stainless steel, 0.007 ± 0.004 mmol iron per year. This equates to a mass loss of 0.054 ± 0.03 mmol iron lost per kilogram stainless steel per year.
- *Fluid residence time in vault* — Hydrologic calculations for the RH-LLW facility indicate that only 10 to 50 pore volumes of water are anticipated to pass through the vault over the 1,000-year performance period. This equates to a residence time within the vault of 20 to 100 years for a given aliquot of water. The median of this range is 60 years residence time.
- *Mass of iron corroded* — Calculations based on above parameters:
  - For carbon steel rebar, there are 310 kg carbon steel per $m^3$ of cracked reinforced concrete with 31% porosity and ~1 kg steel per kg water. This would corrode approximately 4.75 moles iron per kilogram aqueous solution over 60 years.

- For carbon steel waste containers, there are 85.4 kg of steel in containers per cubic meter of vault space. This would corrode approximately 415 moles iron per $m^3$ vault space over 60 years. At 10% moisture (100 L solution per $m^3$), approximately 4.15 moles of iron in carbon steel would corrode per liter of solution, over a 60-year period.
- For stainless steel waste containers, the same boundary conditions exist. However, because stainless steel corrodes more slowly, less than 0.003 moles moles iron per kilogram aqueous solution would corrode over 60 years

## A-8. Waste Forms Inside Liner

After water infiltrates through the steel liners, it will encounter three types of waste forms: (1) anion-exchange resins, (2) corroding metal reactor parts, and (3) miscellaneous debris. The influent solution for this step is the effluent solution from the corrosion of steel liners. Model calculations involving the reaction of this influent water with steel are founded on the following assumptions:

- Miscellaneous debris is assumed to be inert
- All reactor parts are assumed to be made of stainless steel or other metals that corrodes at the carbon steel rates provided by Adler-Flitton (2004)
- The annual release rate of iron into solution is assumed to be linear (e.g., $0^{th}$ order)
- Anion-exchange resins are assumed to have no chemical selectivity.

The model treats stainless steel reactor parts in the same way it treats stainless steel liners (above). The only difference is in the total mass of corroding steel. The mass of iron released into the system over a 60-year period is estimated as follows:

- Total mass of stainless steel, zircalloy, NiCrFe-alloy parts estimated to be sent to the NRF section of the RH-LLW facility is 862,727 kg (Jeff Sondrup, personal communication).
- Along with carbon steel waste containers whose impact on solution chemistry has already been estimated, these parts will be stored in approximately 240,000 $ft^3$ of vault space.
- The NRF portion of the RH-LLW facility is assumed to be emulative of the overall facility. Other sections will contain some aluminum, but the overall percentage of aluminum in the RH-LLW facility is less than 0.5%. Aluminum is assumed to be negligible.
- From this data, there are an estimated 3.6 kg of stainless steel mass per $ft^3$ of vault space or 128.6 kg stainless steel per $m^3$ of vault space.
- Assume a maximum of 10% of total vault space contains water. This equates to 100 L solution per $m^3$ of vault space.
- End result, based on Adler-Flitton's corrosion data (0.054 ± 0.03 mmol iron lost per kilogram stainless steel per year), is 0.42 moles of iron in stainless steel lost per liter of solution in the vault over 60 years.

## A-9. Vault Floor and Sand/Gravel Base

Contaminated water leaving the waste containers will encounter the bottom of the vault. This structure will be similar to the top, except that it also will have drainage holes to prevent the vault from flooding. Thus, exiting water will travel over surfaces rather than through cracks. The model also assumes that the surfaces of the cement in the bottom of the vault will have been exposed to water for longer than the cracks that form in the top of the vault; therefore, all cement will either be mature or degraded. The PHREEQc calculations here assume the same physical composition as in the top of the vault, but replace the fresh cement used there with mature or degraded cement. Effluent from the bottom of the vault will comprise part of the influent solution for the vault underlayment.

The vault underlayment is assumed to have two sources of influent solution: (1) effluent from the bottom of the vault and (2) native alluvium water. The mixing proportion for these two solutions ranges from 50/50 to 95% vault 5% alluvium. All mixing between vault exit water and native alluvium water is assumed to occur in the vault underlayment. The vault underlayment is assumed to consist of a mixture of sand (75%) and gravel (25%). This sand/gravel mix is assumed to have a bulk density of 1,875 kg/m$^3$, porosity of 0.5, and 10% moisture content. Sand is modeled as a mix of 75% quartz, 25% amorphous silica, and trace calcite. Granite is modeled as a mix of 70% quartz, 15% albite, and 15% K-feldspar. All calculations assumed water in equilibrium with soil gas (pCO2) and either mature or degraded cement.

## A-10. Underlying Alluvium Sediment

Effluent from the vault underlayment is assumed to provide influent solution for the underlying alluvium. Sediment in the RH-LLW alluvium is anticipated to fall within the compositional range of surficial sediment located elsewhere in INL. In general, INL surficial sediment is a calcareous silty-clay under the unified soil classification system. The grain size distribution is variable. For fine-grained sediment, most samples have 35 to 75% (by mass) within the silt size fraction. Depending on sample and extraction method used, surficial sediment contains 0.3 to 6 mg iron-oxide iron per gram of sediment. Prior x-ray diffraction analyses (Fox et al. 2004, Plummer et al. 2004) have indicated that samples of INL surficial sediment are 50 to 75% quartz, 10 to 25% plagioclase and K-feldspar, 10 to 20% clay minerals, less than 5% olivine and pyroxene, less than 5% calcite, and less than 5% iron oxides. The fine grain size fraction (less than 75 μm) is approximately 40 to 55% quartz, 30 to 45% clay minerals, 5 to 10% plagioclase and K-feldspar, 5 to 10% calcite, and less than 5% iron oxides with trace amounts of gypsum and other minerals. The clay minerals are predominantly mixed illite-smectite (50 to 75%), with kaolinite, illite, and Ca-rich smectite comprising the remaining fraction.

### A-10.1 Data Inputs and Sample Results

Batch mode calculations in PHREEQc require three types of inputs: (1) thermodynamic data, (2) kinetic data, and (3) mass of system components per unit of water. Thermodynamic data are read from a data file, while mass and kinetic data are input as user-defined parameters. These calculations used the same thermodynamic data for all model runs, but have different mass and kinetic parameters. Data inputs are provided for the thermodynamic dataset (as modified). Input parameters and sample results are provided for each of the runs. Thermodynamic data is provided first, and then the input parameters and sample results are aggregated according to the relevant system component. Hopefully, this presentation facilitates comparison between modeling assumptions, parameter inputs, and sample results.

## A-11. Thermodynamic Data

PHREEQc provides a number of standardized thermodynamic datasets. These datasets are each several hundred pages in length, and can be downloaded from the PHREEQc website maintained by the United States Geological Survey (http://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqc/). This study used the "llnl.dat" database and was modified to include cement minerals. The thermodynamic constants used for cement minerals were culled from the literature and manually recalculated to be consistent with the component base species used by PHREEQc. Ten mineral phases were added to the "llnl.dat" data file. These were as follows:

```
CSH(1.0-2.5)
      CaH2SiO4 + 2.000 H+ =  + 1.0000 Ca++ + 1.0000 SiO2 + 2.000 H2O
       log_k        14.8
      -delta_H     0

 #  CSH for cement with Ca/Si ratio = 1.5 (Berner, Waste Mgmt, 1992, vol 12), translated to PHREEQ component base with SiO2 +
2H2O --> H2SiO4 + 2H+
 # Enthalpy of formation:     0 kcal/mol
```

```
Ca(OH)2*(CSH(1.5))
      Ca(OH)2 +2.000 H+ =  + 1.0000 Ca++ + 2.0000 H2O
       log_k        22.277
       -delta_H           0

#     CSH for cement with Ca/Si ratio = 1.5 (Berner, Waste Mgmt, 1992, vol 12)
#     Enthalpy of formation:0 kcal/mol

Ca(OH)2*(CSH(1.8))
      Ca(OH)2 +2.000 H+ =  + 1.0000 Ca++ + 2.0000 H2O
       log_k          22.441
       -delta_H    0

#     CSH for cement with Ca/Si ratio = 1.5 (Berner, Waste Mgmt, 1992, vol 12)
#     Enthalpy of formation:0 kcal/mol


CSH(0.25)
      CaH2SiO4 + 2.000 H+ =  + 1.0000 Ca++ + 1.0000 SiO2 + 2.000 H2O
       log_k          14.96
       -delta_H        0

#     CSH for cement with Ca/Si ratio = 0.5 (Berner, Waste Mgmt, 1992, vol 12)
#     Enthalpy of formation:   0 kcal/mol

SiO2*(CSH(0.25))
       SiO2  =  + 1.0000 SiO2
       log_k          -2.87
-delta_H              0

#     CSH for cement with Ca/Si ratio = 0.5 (Berner, Waste Mgmt, 1992, vol 12)
#     Enthalpy of formation:   0 kcal/mol

NaOH(cement)
       NaOH + 1.000 H+  =  + 1.0000 Na+ + 1.000 H2O
       log_k          14.18
       -delta_H       0

#     From Lothenbach & Winnefeld, Cement and Conc. Res., 2006
#     Enthalpy of formation:   0 kcal/mol

KOH(cement)
       KOH + 1.000 H+  =  + 1.0000 K+ + 1.000 H2O
       log_k          14.46
       -delta_H        0

#     From Lothenbach & Winnefeld, Cement and Conc. Res., 2006
#     Enthalpy of formation:  0 kcal/mol

Hydrogarnet(C3AH6)
      Ca3Al2O6:6H2O + 12.000 H+ = + 3.000 Ca++ + 2.000 Al+++ + 12.000 H2O
       log_k          78.18
       -delta_H        0

#     From (Reardon, Waste Mgmt, 1992, vol 12)
#     Enthalpy of formation:  0 kcal/mol

Glaserite
      K3Na(SO4)2 = + 3.000 K+  + 1.000 Na+  + 2.000 SO4--
       log_k          -3.8
    -delta_H         0
```

```
#    From (Reardon, Waste Mgmt, 1992, vol 12)
#    Enthalpy of formation:  0 kcal/mol

Monosulfate
  Ca4Al2O6SO4:12H2O + 12.000 H+ = + 4.000 Ca++ + 1.000 SO4-- + 18.000 H2O + 2.000 Al+++
      log_k          -3.8
   -delta_H          0

#    From (Reardon, Waste Mgmt, 1992, vol 12)
#    Enthalpy of formation:  0 kcal/mol
```

It is important to note that the cement mineral thermodynamic data used is not likely to be internally consistent with data for (1) other cement mineral phases specified and (2) other thermodynamic data in the llnl.dat data file. Derivation of thermodynamic parameters is a devilishly tricky business because most data for complex reactions is calculated from a combination of experimental measurements and thermodynamic data for the reacting species as defined by the person making the measurements. There is not a defined "standard dataset" for thermodynamic data, and different researchers will select different data for reacting species. Thus, different thermodynamic values in a dataset may be based on different base data for the reacting species (e.g., more than one value for the dissociation constant for water). This limits the accuracy of thermodynamic calculations, unless extreme care is taken to assemble an internally consistent dataset. This thermodynamic data inputs to this model were not parsed to generate an internally consistent dataset, and the model results should be treated accordingly. The calculations only produce first-order estimates.

## A-12. Infiltrating Water and Soil Cap

No modeling calcuations were conducted on this component. Field data were gathered and then two infiltration scenarios were considered for each potential composition of the vault ceiling: (1) minimum concentration of each ion observed, and (2) maximum of each ion concentration observed. These two scenarios bound the minimum and maximum ion concentration that would likely encounter the vault ceiling as long as soil and climactic conditions reflect historical norms. Input data for the model comes from Table 2.

## A-13. Repository Vault (Ceiling)

In order to bound the anticpated infiltration scenarios for groundwater interaction with cement, a total of ten model calculations were conducted. These ten calculations were conducted with ten input files. The output for the fresh cement and mature cement with rebar input files was used as solution inputs for subsequent calculations to evaluate the corrosion of steel liners.

1. Fresh cement (four input files)
   - Minimum ion content, no rebar (file 1)
   - Minimum ion content, with rebar (file 2)
   - Maximum ion content, no rebar (file 3)
   - Maximum ion content, with rebar (file 4)
2. Mature cement (four input files)
   - Minimum ion content, no rebar (file 5)
   - Minimum ion content, with rebar (file 6)
   - Maximum ion content, no rebar (file 7)
   - Maximum ion content, with rebar (file 8)
3. Degraded cement (two input files)

- Minimum ion content, no rebar (file 9)
- Maximum ion content, no rebar (file 10)

Model inputs and results will be presented in order of this file listing. First the input file will be given and then sample results. Phase assemblage and solution composition will be given for the initial condition. These parameters, as well as the distribution of species, will be given for the final time step. Saturation indices were not used in the $K_d$ analyes and are not given.

**File 1. Fresh Cement, Minimum Ion Content, No Rebar**

*INPUT FILE*

```
SOLUTION 1
   temp      15
   pH        7.5
   pe        4
   redox     pe
   units     mmol/kgw
   density   1
   Alkalinity 0
   Cl(-1)    0
   Li        1e-010
   Al        1e-010
   Ca        0.6
   Mg        0.3
   Na        1.3
   K         0
   S(6)      0.3
   N(5)      0
   C(4)      1.4
   Br(-1)    0
   Si        0.01
   -water    1 # kg

GAS_PHASE 1
   -fixed_pressure
   -pressure 1
   -volume 1000
   -temperature 25
   CO2(g)    0.056
   O2(g)     0.18
EQUILIBRIUM_PHASES 1
   Brucite   0 1.39
   Ca(OH)2*(CSH(1.5)) 0 9.5
   Calcite   0 0.001
   CSH(1.0-2.5) 0 15.96
   Gibbsite  0 0.001
   goethite  0 1e-005
   KOH(cement) 0 0.99
   NaOH(cement) 0 0.15
   SiO2(am)  0 0.02
SAVE solution 1-1
END
USE solution 1
GAS_PHASE 2
   -fixed_pressure
   -pressure 1
   -volume 1000
   -temperature 25
   CO2(g)    0.056
   O2(g)     0.18
EQUILIBRIUM_PHASES 2
```

```
   calcite   0 1e-010
   Fe(OH)3   0 1e-010
   goethite  0 1e-010
   portlandite 0 1e-010
   SiO2(am)  0 1e-010
REACTION 3
   Fe        1
   0.025 moles in 60 steps
```

## *SAMPLE OUTPUT, INITIAL CONDITION (FILE 1)*

```
-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 1.

-----------------------------Solution composition------------------------------

      Elements          Molality       Moles

      Al              1.000e-013  1.000e-013
      C(4)             1.400e-003  1.400e-003
      Ca               6.000e-004  6.000e-004
      Li              1.000e-013  1.000e-013
      Mg               3.000e-004  3.000e-004
      Na               1.300e-003  1.300e-003
      S(6)             3.000e-004  3.000e-004
      Si              1.000e-005  1.000e-005

----------------------------Description of solution----------------------------

                                pH  =   7.500
                                pe  =   4.000
                    Activity of water  =   1.000
                       Ionic strength  =  3.581e-003
                      Mass of water (kg)  =  1.000e+000
                Total alkalinity (eq/kg)  =  1.301e-003
                    Total CO2 (mol/kg)  =  1.400e-003
                   Temperature (deg C)  =  15.000
                 Electrical balance (eq)  =  1.199e-003
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  24.59
                          Iterations  =   4
                            Total H  = 1.110519e+002
                            Total O  = 5.553064e+001
```

## *SAMPLE OUTPUT, FINAL TIME STEP (FILE 1)*

```
 -------------------------------------------
Beginning of batch-reaction calculations.
-------------------------------------------

Reaction step 1.

WARNING: Maximum iterations exceeded, 100

WARNING: Numerical method failed with this set of convergence parameters.

WARNING: Trying smaller step size, pe step size 10, 5 ...

WARNING: Maximum iterations exceeded, 200
```

WARNING: Numerical method failed with this set of convergence parameters.

WARNING: Trying reduced tolerance 1e-016 ...

Using solution 1.
Using pure phase assemblage 1.
Using gas phase 1.

----------Gas phase----------

Total pressure: 1.0000 atmospheres
Gas volume: 1.74e+002 liters

| | | | Moles in gas | | |
|---|---|---|---|---|---|
| Component | log P | P | Initial | Final | Delta |
| CO2(g) | -12.55 | 2.851e-013 | 2.289e+000 | 2.097e-012 | -2.289e+000 |
| O2(g) | -0.00 | 1.000e+000 | 7.357e+000 | 7.356e+000 | -1.285e-003 |

----------Phase assemblage----------

| | | | Moles in assemblage | | |
|---|---|---|---|---|---|
| Phase | SI | log IAP log KT | Initial | Final | Delta |
| Brucite | 0.00 | 16.96 16.96 | 1.390e+000 | 1.390e+000 | 3.000e-004 |
| Ca(OH)2*(CSH(1.5)) | 0.00 | 22.28 22.28 | 9.500e+000 | 7.243e+000 | -2.257e+000 |
| Calcite | 0.00 | 1.98 1.98 | 1.000e-003 | 2.275e+000 | 2.274e+000 |
| CSH(1.0-2.5) | 0.00 | 14.80 14.80 | 1.596e+001 | 1.594e+001 | -1.635e-002 |
| Gibbsite | -1.67 | 6.69 8.36 | 1.000e-003 | 0 | -1.000e-003 |
| Goethite | 0.00 | 0.91 0.91 | 1.000e-005 | 9.643e-006 | -3.564e-007 |
| KOH(cement) | -0.73 | 13.73 14.46 | 9.900e-001 | 0 | -9.900e-001 |
| NaOH(cement) | -1.17 | 13.01 14.18 | 1.500e-001 | 0 | -1.500e-001 |
| SiO2(am) | -4.60 | -7.48 -2.87 | 2.000e-002 | 0 | -2.000e-002 |

----------Solution composition----------

| Elements | Molality | Moles |
|---|---|---|
| Al | 9.604e-004 | 1.000e-003 |
| C | 1.591e-002 | 1.657e-002 |
| Ca | 4.720e-005 | 4.915e-005 |
| Fe | 3.424e-007 | 3.565e-007 |
| K | 9.507e-001 | 9.900e-001 |
| Li | 9.604e-014 | 1.000e-013 |
| Mg | 3.786e-011 | 3.943e-011 |
| Na | 1.453e-001 | 1.513e-001 |
| S | 2.881e-004 | 3.000e-004 |
| Si | 3.491e-002 | 3.636e-002 |

----------Description of solution----------

pH = 14.079 Charge balance
pe = 7.456 Adjusted to redox equilibrium
Activity of water = 0.967
Ionic strength = 9.441e-001
Mass of water (kg) = 1.041e+000
Total alkalinity (eq/kg) = 1.097e+000
Total CO2 (mol/kg) = 1.591e-002
Temperature (deg C) = 15.000
Electrical balance (eq) = 1.199e-003

```
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   0.06
                        Iterations  =  89
                          Total H  = 1.167407e+002
                          Total O  = 5.905125e+001

----------------------------Distribution of species----------------------------

                                      Log      Log       Log
  Species              Molality    Activity  Molality  Activity    Gamma

  OH-                 7.982e-001  5.100e-001    -0.098    -0.292    -0.195
  H+                  1.025e-014  8.342e-015   -13.989   -14.079    -0.090
  H2O                 5.553e+001  9.669e-001     1.744    -0.015     0.000
Al            9.604e-004
  AlO2-               9.510e-004  6.308e-004    -3.022    -3.200    -0.178
  NaAlO2              9.353e-006  9.353e-006    -5.029    -5.029     0.000
  HAlO2               2.563e-011  2.563e-011   -10.591   -10.591     0.000
  Al(OH)2+            4.234e-019  2.808e-019   -18.373   -18.552    -0.178
  AlOH+2              1.210e-026  2.061e-027   -25.917   -26.686    -0.769
  Al+3                4.027e-035  3.166e-036   -34.395   -35.499    -1.104
  AlSO4+              1.081e-037  7.167e-038   -36.966   -37.145    -0.178
  Al(SO4)2-           1.856e-040  1.231e-040   -39.732   -39.910    -0.178
  Al2(OH)2+4          0.000e+000  0.000e+000   -47.746   -50.561    -2.814
  Al3(OH)4+5          0.000e+000  0.000e+000   -59.947   -64.122    -4.175
  Al13O4(OH)24+7      0.000e+000  0.000e+000  -101.894  -110.113    -8.219
C(-2)         0.000e+000
  C2H4                0.000e+000  0.000e+000  -295.853  -295.853     0.000
C(-3)         0.000e+000
  C2H6                0.000e+000  0.000e+000  -267.718  -267.718     0.000
C(-4)         0.000e+000
  CH4                 0.000e+000  0.000e+000  -164.044  -164.044     0.000
C(2)          0.000e+000
  CO                  0.000e+000  0.000e+000   -62.249   -62.249     0.000
C(4)          1.591e-002
  CO3-2               1.441e-002  2.454e-003    -1.841    -2.610    -0.769
  NaCO3-              1.491e-003  9.887e-004    -2.827    -3.005    -0.178
  CaCO3               6.322e-006  6.322e-006    -5.199    -5.199     0.000
  HCO3-               8.582e-007  5.692e-007    -6.066    -6.245    -0.178
  NaHCO3              8.770e-008  8.770e-008    -7.057    -7.057     0.000
  MgCO3               1.540e-011  1.540e-011   -10.813   -10.813     0.000
  CaHCO3+             1.412e-011  9.365e-012   -10.850   -11.028    -0.178
  CO2                 1.058e-014  1.321e-014   -13.976   -13.879     0.096
  MgHCO3+             6.668e-017  4.423e-017   -16.176   -16.354    -0.178
  FeCO3               4.364e-034  4.364e-034   -33.360   -33.360     0.000
  FeCO3+              2.682e-034  1.779e-034   -33.571   -33.750    -0.178
  FeHCO3+             1.144e-039  7.586e-040   -38.942   -39.120    -0.178
Ca            4.720e-005
  CaOH+               3.477e-005  2.306e-005    -4.459    -4.637    -0.178
  CaCO3               6.322e-006  6.322e-006    -5.199    -5.199     0.000
  Ca+2                6.101e-006  1.409e-006    -5.215    -5.851    -0.637
  CaSO4               4.156e-009  4.156e-009    -8.381    -8.381     0.000
  CaHCO3+             1.412e-011  9.365e-012   -10.850   -11.028    -0.178
Fe(2)         9.029e-025
  Fe(OH)3-            5.963e-025  3.955e-025   -24.225   -24.403    -0.178
  Fe(OH)4-2           3.066e-025  4.584e-026   -24.513   -25.339    -0.825
  Fe(OH)2             8.570e-029  8.570e-029   -28.067   -28.067     0.000
  FeOH+               1.403e-031  9.308e-032   -30.853   -31.031    -0.178
  FeCO3               4.364e-034  4.364e-034   -33.360   -33.360     0.000
  Fe+2                1.100e-035  2.540e-036   -34.959   -35.595    -0.637
  FeSO4               8.904e-039  8.904e-039   -38.050   -38.050     0.000
  FeHCO3+             1.144e-039  7.586e-040   -38.942   -39.120    -0.178
Fe(3)         3.424e-007
```

| | | | | | |
|---|---|---|---|---|---|
| Fe(OH)4- | 3.424e-007 | 2.271e-007 | -6.465 | -6.644 | -0.178 |
| Fe(OH)3 | 7.800e-012 | 7.800e-012 | -11.108 | -11.108 | 0.000 |
| Fe(OH)2+ | 2.169e-019 | 1.439e-019 | -18.664 | -18.842 | -0.178 |
| FeOH+2 | 2.202e-029 | 3.749e-030 | -28.657 | -29.426 | -0.769 |
| FeCO3+ | 2.682e-034 | 1.779e-034 | -33.571 | -33.750 | -0.178 |
| Fe+3 | 0.000e+000 | 0.000e+000 | -40.196 | -41.300 | -1.104 |
| FeSO4+ | 0.000e+000 | 0.000e+000 | -43.956 | -44.134 | -0.178 |
| Fe(SO4)2- | 0.000e+000 | 0.000e+000 | -47.219 | -47.397 | -0.178 |
| Fe2(OH)2+4 | 0.000e+000 | 0.000e+000 | -54.608 | -57.422 | -2.814 |
| Fe3(OH)4+5 | 0.000e+000 | 0.000e+000 | -69.769 | -73.944 | -4.175 |
| H(0) | 0.000e+000 | | | | |
| H2 | 0.000e+000 | 0.000e+000 | -46.474 | -46.378 | 0.096 |
| K | 9.507e-001 | | | | |
| K+ | 7.630e-001 | 4.668e-001 | -0.117 | -0.331 | -0.213 |
| KOH | 1.876e-001 | 1.876e-001 | -0.727 | -0.727 | 0.000 |
| KSO4- | 1.205e-004 | 7.995e-005 | -3.919 | -4.097 | -0.178 |
| KHSO4 | 4.052e-019 | 4.052e-019 | -18.392 | -18.392 | 0.000 |
| Li | 9.604e-014 | | | | |
| LiOH | 6.362e-014 | 6.362e-014 | -13.196 | -13.196 | 0.000 |
| Li+ | 3.241e-014 | 2.396e-014 | -13.489 | -13.621 | -0.131 |
| LiSO4- | 4.706e-018 | 3.121e-018 | -17.327 | -17.506 | -0.178 |
| Mg | 3.786e-011 | | | | |
| Mg+2 | 2.243e-011 | 6.843e-012 | -10.649 | -11.165 | -0.516 |
| MgCO3 | 1.540e-011 | 1.540e-011 | -10.813 | -10.813 | 0.000 |
| MgSO4 | 3.105e-014 | 3.105e-014 | -13.508 | -13.508 | 0.000 |
| MgHCO3+ | 6.668e-017 | 4.423e-017 | -16.176 | -16.354 | -0.178 |
| Mg4(OH)4+4 | 4.590e-026 | 7.037e-029 | -25.338 | -28.153 | -2.814 |
| Na | 1.453e-001 | | | | |
| Na+ | 1.342e-001 | 8.899e-002 | -0.872 | -1.051 | -0.178 |
| NaOH | 8.025e-003 | 8.025e-003 | -2.096 | -2.096 | 0.000 |
| NaHSiO3 | 1.590e-003 | 1.590e-003 | -2.799 | -2.799 | 0.000 |
| NaCO3- | 1.491e-003 | 9.887e-004 | -2.827 | -3.005 | -0.178 |
| NaSO4- | 1.961e-005 | 1.301e-005 | -4.708 | -4.886 | -0.178 |
| NaAlO2 | 9.353e-006 | 9.353e-006 | -5.029 | -5.029 | 0.000 |
| NaHCO3 | 8.770e-008 | 8.770e-008 | -7.057 | -7.057 | 0.000 |
| O(0) | 2.468e-003 | | | | |
| O2 | 1.234e-003 | 1.541e-003 | -2.909 | -2.812 | 0.096 |
| S(-2) | 0.000e+000 | | | | |
| S-2 | 0.000e+000 | 0.000e+000 | -155.088 | -155.807 | -0.719 |
| HS- | 0.000e+000 | 0.000e+000 | -156.465 | -156.659 | -0.195 |
| H2S | 0.000e+000 | 0.000e+000 | -163.587 | -163.587 | 0.000 |
| S2-2 | 0.000e+000 | 0.000e+000 | -279.308 | -280.133 | -0.825 |
| S3-2 | 0.000e+000 | 0.000e+000 | -403.670 | -404.496 | -0.825 |
| S4-2 | 0.000e+000 | 0.000e+000 | -528.264 | -529.090 | -0.825 |
| S5-2 | 0.000e+000 | 0.000e+000 | -653.084 | -653.909 | -0.825 |
| S(2) | 0.000e+000 | | | | |
| S2O3-2 | 0.000e+000 | 0.000e+000 | -169.675 | -170.500 | -0.825 |
| HS2O3- | 0.000e+000 | 0.000e+000 | -183.387 | -183.565 | -0.178 |
| S(3) | 0.000e+000 | | | | |
| S2O4-2 | 0.000e+000 | 0.000e+000 | -155.428 | -156.148 | -0.719 |
| S(4) | 0.000e+000 | | | | |
| SO3-2 | 0.000e+000 | 0.000e+000 | -50.726 | -51.495 | -0.769 |
| HSO3- | 0.000e+000 | 0.000e+000 | -58.217 | -58.395 | -0.178 |
| H2SO3 | 0.000e+000 | 0.000e+000 | -70.439 | -70.439 | 0.000 |
| SO2 | 0.000e+000 | 0.000e+000 | -70.678 | -70.678 | 0.000 |
| S2O6-2 | 0.000e+000 | 0.000e+000 | -88.755 | -89.581 | -0.825 |
| S3O6-2 | 0.000e+000 | 0.000e+000 | -215.647 | -216.473 | -0.825 |
| S4O6-2 | 0.000e+000 | 0.000e+000 | -326.274 | -327.099 | -0.825 |
| S5O6-2 | 0.000e+000 | 0.000e+000 | -466.405 | -467.231 | -0.825 |
| S(5) | 0.000e+000 | | | | |
| S2O5-2 | 0.000e+000 | 0.000e+000 | -120.760 | -121.586 | -0.825 |
| S(6) | 2.881e-004 | | | | |

```
   SO4-2              1.480e-004  2.212e-005    -3.830    -4.655    -0.825
   KSO4-              1.205e-004  7.995e-005    -3.919    -4.097    -0.178
   NaSO4-             1.961e-005  1.301e-005    -4.708    -4.886    -0.178
   CaSO4              4.156e-009  4.156e-009    -8.381    -8.381     0.000
   MgSO4              3.105e-014  3.105e-014   -13.508   -13.508     0.000
   HSO4-              2.122e-017  1.407e-017   -16.673   -16.852    -0.178
   LiSO4-             4.706e-018  3.121e-018   -17.327   -17.506    -0.178
   KHSO4              4.052e-019  4.052e-019   -18.392   -18.392     0.000
   H2SO4              1.467e-034  1.467e-034   -33.834   -33.834     0.000
   AlSO4+             1.081e-037  7.167e-038   -36.966   -37.145    -0.178
   FeSO4              8.904e-039  8.904e-039   -38.050   -38.050     0.000
   Al(SO4)2-          1.856e-040  1.231e-040   -39.732   -39.910    -0.178
   FeSO4+             0.000e+000  0.000e+000   -43.956   -44.134    -0.178
   Fe(SO4)2-          0.000e+000  0.000e+000   -47.219   -47.397    -0.178
S(7)          0.000e+000
   S2O8-2             0.000e+000  0.000e+000   -61.672   -62.497    -0.825
S(8)          8.478e-039
   HSO5-              8.478e-039  5.623e-039   -38.072   -38.250    -0.178
Si            3.491e-002
   H2SiO4-2           3.285e-002  4.912e-003    -1.483    -2.309    -0.825
   NaHSiO3            1.590e-003  1.590e-003    -2.799    -2.799     0.000
   HSiO3-             4.704e-004  3.120e-004    -3.328    -3.506    -0.178
   H4(H2SiO4)4-4      5.800e-007  2.239e-010    -6.237    -9.650    -3.413
   SiO2               3.334e-008  3.334e-008    -7.477    -7.477     0.000
   H6(H2SiO4)4-2      2.080e-015  3.109e-016   -14.682   -15.507    -0.825
```

## FILE 2. Fresh Cement, Minimum Ion Content, With Rebar

*INPUT FILE*

```
SOLUTION 1
    temp      15
    pH        7.5
    pe        4
    redox     pe
    units     mmol/kgw
    density   1
    Alkalinity 0
    Cl(-1)    0
    Li        1e-010
    Al        1e-010
    Ca        0.6
    Mg        0.3
    Na        1.3
    K         0
    S(6)      0.3
    N(5)      0
    C(4)      1.4
    Br(-1)    0
    Si        0.01
    -water    1 # kg

GAS_PHASE 1
    -fixed_pressure
    -pressure 1
    -volume 1000
    -temperature 25
    CO2(g)    0.056
    O2(g)     0.18
EQUILIBRIUM_PHASES 1
    Brucite   0 1.39
    Ca(OH)2*(CSH(1.5)) 0 9.5
```

```
    Calcite   0 0.001
    CSH(1.0-2.5) 0 15.96
    Gibbsite  0 0.001
    goethite  0 1e-005
    KOH(cement) 0 0.99
    NaOH(cement) 0 0.15
    SiO2(am)  0 0.02
REACTION 1
    Fe        1
    4.75 moles in 60 steps
SAVE solution 1-1
END
```

## *SAMPLE OUTPUT, INITIAL CONDITION (FILE 2)*

```
-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 1.

-----------------------------Solution composition------------------------------

      Elements          Molality       Moles

      Al             1.000e-013  1.000e-013
      C(4)            1.400e-003  1.400e-003
      Ca              6.000e-004  6.000e-004
      Li             1.000e-013  1.000e-013
      Mg              3.000e-004  3.000e-004
      Na              1.300e-003  1.300e-003
      S(6)            3.000e-004  3.000e-004
      Si             1.000e-005  1.000e-005

----------------------------Description of solution----------------------------

                                pH  =  7.500
                                pe  =  4.000
                    Activity of water  =  1.000
                       Ionic strength  =  3.581e-003
                   Mass of water (kg)  =  1.000e+000
              Total alkalinity (eq/kg)  =  1.301e-003
                  Total CO2 (mol/kg)  =  1.400e-003
                 Temperature (deg C)  =  15.000
               Electrical balance (eq)  =  1.199e-003
Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  24.59
                           Iterations  =  4
                             Total H  = 1.110519e+002
                             Total O  = 5.553064e+001
```

## *SAMPLE OUTPUT, FINAL TIME STEP (FILE 2)*

```
Reaction step 60.

Using solution 1.
Using pure phase assemblage 1.
Using gas phase 1.
Using reaction 1.

Reaction 1.       Irreversible reaction defined in simulation 1.

      4.750e+000 moles of the following reaction have been added:
```

| Reactant | Relative moles |
|---|---|
| Fe | 1.00000 |

| Element | Relative moles |
|---|---|
| Fe | 1.00000 |

----------Gas phase----------

Total pressure: 1.0000 atmospheres
Gas volume: 8.97e+001 liters

| Component | log P | P | Moles in gas Initial | Final | Delta |
|---|---|---|---|---|---|
| CO2(g) | -12.55 | 2.847e-013 | 2.289e+000 | 1.080e-012 | -2.289e+000 |
| O2(g) | -0.00 | 1.000e+000 | 7.357e+000 | 3.793e+000 | -3.564e+000 |

----------Phase assemblage----------

| Phase | SI | log IAP | log KT | Moles in assemblage Initial | Final | Delta |
|---|---|---|---|---|---|---|
| Brucite | 0.00 | 16.96 | 16.96 | 1.390e+000 | 1.390e+000 | 3.000e-004 |
| Ca(OH)2*(CSH(1.5)) | 0.00 | 22.28 | 22.28 | 9.500e+000 | 7.245e+000 | -2.255e+000 |
| Calcite | 0.00 | 1.98 | 1.98 | 1.000e-003 | 2.274e+000 | 2.273e+000 |
| CSH(1.0-2.5) | 0.00 | 14.80 | 14.80 | 1.596e+001 | 1.594e+001 | -1.752e-002 |
| Gibbsite | -1.67 | 6.70 | 8.36 | 1.000e-003 | 0 | -1.000e-003 |
| Goethite | -0.00 | 0.91 | 0.91 | 1.000e-005 | 4.750e+000 | 4.750e+000 |
| KOH(cement) | -0.70 | 13.76 | 14.46 | 9.900e-001 | 0 | -9.900e-001 |
| NaOH(cement) | -1.14 | 13.04 | 14.18 | 1.500e-001 | 0 | -1.500e-001 |
| SiO2(am) | -4.60 | -7.48 | -2.87 | 2.000e-002 | 0 | -2.000e-002 |

----------Solution composition----------

| Elements | Molality | Moles |
|---|---|---|
| Al | 1.001e-003 | 1.000e-003 |
| C | 1.715e-002 | 1.713e-002 |
| Ca | 4.585e-005 | 4.579e-005 |
| Fe | 3.529e-007 | 3.523e-007 |
| K | 9.915e-001 | 9.900e-001 |
| Li | 1.001e-013 | 1.000e-013 |
| Mg | 3.660e-011 | 3.655e-011 |
| Na | 1.515e-001 | 1.513e-001 |
| S | 3.004e-004 | 3.000e-004 |
| Si | 3.759e-002 | 3.753e-002 |

----------Description of solution----------

pH = 14.093 Charge balance
pe = 7.442 Adjusted to redox equilibrium
Activity of water = 0.966
Ionic strength = 9.813e-001
Mass of water (kg) = 9.985e-001
Total alkalinity (eq/kg) = 1.144e+000
Total CO2 (mol/kg) = 1.715e-002

Temperature (deg C) = 15.000
Electrical balance (eq) = 1.199e-003
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 0.06
Iterations = 53
Total H = 1.119895e+002
Total O = 5.667904e+001

----------Distribution of species----------

| Species | Molality | Log Activity | Log Molality | Log Activity | Gamma |
|---|---|---|---|---|---|
| OH- | 8.242e-001 | 5.258e-001 | -0.084 | -0.279 | -0.195 |
| H+ | 9.910e-015 | 8.080e-015 | -14.004 | -14.093 | -0.089 |
| H2O | 5.553e+001 | 9.656e-001 | 1.744 | -0.015 | 0.000 |
| Al | 1.001e-003 | | | | |
| AlO2- | 9.914e-004 | 6.570e-004 | -3.004 | -3.182 | -0.179 |
| NaAlO2 | 1.012e-005 | 1.012e-005 | -4.995 | -4.995 | 0.000 |
| HAlO2 | 2.586e-011 | 2.586e-011 | -10.587 | -10.587 | 0.000 |
| Al(OH)2+ | 4.140e-019 | 2.744e-019 | -18.383 | -18.562 | -0.179 |
| AlOH+2 | 1.160e-026 | 1.953e-027 | -25.935 | -26.709 | -0.774 |
| Al+3 | 3.737e-035 | 2.910e-036 | -34.427 | -35.536 | -1.109 |
| AlSO4+ | 1.012e-037 | 6.705e-038 | -36.995 | -37.174 | -0.179 |
| Al(SO4)2- | 1.768e-040 | 1.172e-040 | -39.752 | -39.931 | -0.179 |
| Al2(OH)2+4 | 0.000e+000 | 0.000e+000 | -47.775 | -50.608 | -2.833 |
| Al3(OH)4+5 | 0.000e+000 | 0.000e+000 | -59.978 | -64.179 | -4.201 |
| Al13O4(OH)24+7 | 0.000e+000 | 0.000e+000 | -101.890 | -110.162 | -8.272 |
| C(-2) | 0.000e+000 | | | | |
| C2H4 | 0.000e+000 | 0.000e+000 | -295.855 | -295.855 | 0.000 |
| C(-3) | 0.000e+000 | | | | |
| C2H6 | 0.000e+000 | 0.000e+000 | -267.721 | -267.721 | 0.000 |
| C(-4) | 0.000e+000 | | | | |
| CH4 | 0.000e+000 | 0.000e+000 | -164.046 | -164.046 | 0.000 |
| C(2) | 0.000e+000 | | | | |
| CO | 0.000e+000 | 0.000e+000 | -62.250 | -62.250 | 0.000 |
| C(4) | 1.715e-002 | | | | |
| CO3-2 | 1.550e-002 | 2.609e-003 | -1.810 | -2.584 | -0.774 |
| NaCO3- | 1.648e-003 | 1.092e-003 | -2.783 | -2.962 | -0.179 |
| CaCO3 | 6.322e-006 | 6.322e-006 | -5.199 | -5.199 | 0.000 |
| HCO3- | 8.844e-007 | 5.861e-007 | -6.053 | -6.232 | -0.179 |
| NaHCO3 | 9.385e-008 | 9.385e-008 | -7.028 | -7.028 | 0.000 |
| MgCO3 | 1.540e-011 | 1.540e-011 | -10.813 | -10.813 | 0.000 |
| CaHCO3+ | 1.369e-011 | 9.071e-012 | -10.864 | -11.042 | -0.179 |
| CO2 | 1.047e-014 | 1.319e-014 | -13.980 | -13.880 | 0.100 |
| MgHCO3+ | 6.464e-017 | 4.284e-017 | -16.190 | -16.368 | -0.179 |
| FeCO3 | 4.362e-034 | 4.362e-034 | -33.360 | -33.360 | 0.000 |
| FeCO3+ | 2.600e-034 | 1.723e-034 | -33.585 | -33.764 | -0.179 |
| FeHCO3+ | 1.108e-039 | 7.342e-040 | -38.955 | -39.134 | -0.179 |
| Ca | 4.585e-005 | | | | |
| CaOH+ | 3.375e-005 | 2.237e-005 | -4.472 | -4.650 | -0.179 |
| CaCO3 | 6.322e-006 | 6.322e-006 | -5.199 | -5.199 | 0.000 |
| Ca+2 | 5.778e-006 | 1.325e-006 | -5.238 | -5.878 | -0.640 |
| CaSO4 | 3.979e-009 | 3.979e-009 | -8.400 | -8.400 | 0.000 |
| CaHCO3+ | 1.369e-011 | 9.071e-012 | -10.864 | -11.042 | -0.179 |
| Fe(2) | 9.451e-025 | | | | |
| Fe(OH)3- | 6.149e-025 | 4.075e-025 | -24.211 | -24.390 | -0.179 |
| Fe(OH)4-2 | 3.301e-025 | 4.870e-026 | -24.481 | -25.312 | -0.831 |
| Fe(OH)2 | 8.564e-029 | 8.564e-029 | -28.067 | -28.067 | 0.000 |
| FeOH+ | 1.361e-031 | 9.022e-032 | -30.866 | -31.045 | -0.179 |
| FeCO3 | 4.362e-034 | 4.362e-034 | -33.360 | -33.360 | 0.000 |
| Fe+2 | 1.041e-035 | 2.387e-036 | -34.983 | -35.622 | -0.640 |
| FeSO4 | 8.519e-039 | 8.519e-039 | -38.070 | -38.070 | 0.000 |

| | | | | | |
|---|---|---|---|---|---|
| FeHCO3+ | 1.108e-039 | 7.342e-040 | -38.955 | -39.134 | -0.179 |
| Fe(3) | 3.529e-007 | | | | |
| Fe(OH)4- | 3.529e-007 | 2.338e-007 | -6.452 | -6.631 | -0.179 |
| Fe(OH)3 | 7.790e-012 | 7.790e-012 | -11.108 | -11.108 | 0.000 |
| Fe(OH)2+ | 2.103e-019 | 1.393e-019 | -18.677 | -18.856 | -0.179 |
| FeOH+2 | 2.092e-029 | 3.521e-030 | -28.679 | -29.453 | -0.774 |
| FeCO3+ | 2.600e-034 | 1.723e-034 | -33.585 | -33.764 | -0.179 |
| Fe+3 | 0.000e+000 | 0.000e+000 | -40.232 | -41.341 | -1.109 |
| FeSO4+ | 0.000e+000 | 0.000e+000 | -43.989 | -44.167 | -0.179 |
| Fe(SO4)2- | 0.000e+000 | 0.000e+000 | -47.243 | -47.422 | -0.179 |
| Fe2(OH)2+4 | 0.000e+000 | 0.000e+000 | -54.644 | -57.477 | -2.833 |
| Fe3(OH)4+5 | 0.000e+000 | 0.000e+000 | -69.811 | -74.013 | -4.201 |
| H(0) | 0.000e+000 | | | | |
| H2 | 0.000e+000 | 0.000e+000 | -46.478 | -46.378 | 0.100 |
| K | 9.915e-001 | | | | |
| K+ | 7.912e-001 | 4.829e-001 | -0.102 | -0.316 | -0.214 |
| KOH | 2.001e-001 | 2.001e-001 | -0.699 | -0.699 | 0.000 |
| KSO4- | 1.270e-004 | 8.419e-005 | -3.896 | -4.075 | -0.179 |
| KHSO4 | 4.133e-019 | 4.133e-019 | -18.384 | -18.384 | 0.000 |
| Li | 1.001e-013 | | | | |
| LiOH | 6.705e-014 | 6.705e-014 | -13.174 | -13.174 | 0.000 |
| Li+ | 3.310e-014 | 2.449e-014 | -13.480 | -13.611 | -0.131 |
| LiSO4- | 4.900e-018 | 3.247e-018 | -17.310 | -17.489 | -0.179 |
| Mg | 3.660e-011 | | | | |
| Mg+2 | 2.118e-011 | 6.436e-012 | -10.674 | -11.191 | -0.517 |
| MgCO3 | 1.540e-011 | 1.540e-011 | -10.813 | -10.813 | 0.000 |
| MgSO4 | 2.973e-014 | 2.973e-014 | -13.527 | -13.527 | 0.000 |
| MgHCO3+ | 6.464e-017 | 4.284e-017 | -16.190 | -16.368 | -0.179 |
| Mg4(OH)4+4 | 4.238e-026 | 6.226e-029 | -25.373 | -28.206 | -2.833 |
| Na | 1.515e-001 | | | | |
| Na+ | 1.395e-001 | 9.248e-002 | -0.855 | -1.034 | -0.179 |
| NaOH | 8.599e-003 | 8.599e-003 | -2.066 | -2.066 | 0.000 |
| NaHSiO3 | 1.703e-003 | 1.703e-003 | -2.769 | -2.769 | 0.000 |
| NaCO3- | 1.648e-003 | 1.092e-003 | -2.783 | -2.962 | -0.179 |
| NaSO4- | 2.076e-005 | 1.376e-005 | -4.683 | -4.861 | -0.179 |
| NaAlO2 | 1.012e-005 | 1.012e-005 | -4.995 | -4.995 | 0.000 |
| NaHCO3 | 9.385e-008 | 9.385e-008 | -7.028 | -7.028 | 0.000 |
| O(0) | 2.447e-003 | | | | |
| O2 | 1.223e-003 | 1.541e-003 | -2.912 | -2.812 | 0.100 |
| S(-2) | 0.000e+000 | | | | |
| S-2 | 0.000e+000 | 0.000e+000 | -155.076 | -155.800 | -0.724 |
| HS- | 0.000e+000 | 0.000e+000 | -156.470 | -156.665 | -0.195 |
| H2S | 0.000e+000 | 0.000e+000 | -163.607 | -163.607 | 0.000 |
| S2-2 | 0.000e+000 | 0.000e+000 | -279.314 | -280.145 | -0.831 |
| S3-2 | 0.000e+000 | 0.000e+000 | -403.696 | -404.527 | -0.831 |
| S4-2 | 0.000e+000 | 0.000e+000 | -528.309 | -529.140 | -0.831 |
| S5-2 | 0.000e+000 | 0.000e+000 | -653.148 | -653.980 | -0.831 |
| S(2) | 0.000e+000 | | | | |
| S2O3-2 | 0.000e+000 | 0.000e+000 | -169.681 | -170.512 | -0.831 |
| HS2O3- | 0.000e+000 | 0.000e+000 | -183.412 | -183.591 | -0.179 |
| S(3) | 0.000e+000 | | | | |
| S2O4-2 | 0.000e+000 | 0.000e+000 | -155.436 | -156.159 | -0.724 |
| S(4) | 0.000e+000 | | | | |
| SO3-2 | 0.000e+000 | 0.000e+000 | -50.714 | -51.487 | -0.774 |
| HSO3- | 0.000e+000 | 0.000e+000 | -58.223 | -58.402 | -0.179 |
| H2SO3 | 0.000e+000 | 0.000e+000 | -70.459 | -70.459 | 0.000 |
| SO2 | 0.000e+000 | 0.000e+000 | -70.697 | -70.697 | 0.000 |
| S2O6-2 | 0.000e+000 | 0.000e+000 | -88.761 | -89.593 | -0.831 |
| S3O6-2 | 0.000e+000 | 0.000e+000 | -215.673 | -216.504 | -0.831 |
| S4O6-2 | 0.000e+000 | 0.000e+000 | -326.318 | -327.150 | -0.831 |
| S5O6-2 | 0.000e+000 | 0.000e+000 | -466.470 | -467.301 | -0.831 |
| S(5) | 0.000e+000 | | | | |

```
   S2O5-2             0.000e+000  0.000e+000  -120.766  -121.598    -0.831
S(6)          3.004e-004
   SO4-2              1.526e-004  2.252e-005    -3.816    -4.647    -0.831
   KSO4-              1.270e-004  8.419e-005    -3.896    -4.075    -0.179
   NaSO4-             2.076e-005  1.376e-005    -4.683    -4.861    -0.179
   CaSO4              3.979e-009  3.979e-009    -8.400    -8.400     0.000
   MgSO4              2.973e-014  2.973e-014   -13.527   -13.527     0.000
   HSO4-              2.093e-017  1.387e-017   -16.679   -16.858    -0.179
   LiSO4-             4.900e-018  3.247e-018   -17.310   -17.489    -0.179
   KHSO4              4.133e-019  4.133e-019   -18.384   -18.384     0.000
   H2SO4              1.401e-034  1.401e-034   -33.854   -33.854     0.000
   AlSO4+             1.012e-037  6.705e-038   -36.995   -37.174    -0.179
   FeSO4              8.519e-039  8.519e-039   -38.070   -38.070     0.000
   Al(SO4)2-          1.768e-040  1.172e-040   -39.752   -39.931    -0.179
   FeSO4+             0.000e+000  0.000e+000   -43.989   -44.167    -0.179
   Fe(SO4)2-          0.000e+000  0.000e+000   -47.243   -47.422    -0.179
S(7)          0.000e+000
   S2O8-2             0.000e+000  0.000e+000   -61.678   -62.509    -0.831
S(8)          8.365e-039
   HSO5-              8.365e-039  5.544e-039   -38.078   -38.256    -0.179
Si            3.759e-002
   H2SiO4-2           3.540e-002  5.222e-003    -1.451    -2.282    -0.831
   NaHSiO3            1.703e-003  1.703e-003    -2.769    -2.769     0.000
   HSiO3-             4.854e-004  3.217e-004    -3.314    -3.493    -0.179
   H4(H2SiO4)4-4      6.951e-007  2.517e-010    -6.158    -9.599    -3.441
   SiO2               3.334e-008  3.334e-008    -7.477    -7.477     0.000
   H6(H2SiO4)4-2      2.223e-015  3.279e-016   -14.653   -15.484    -0.831
```

## FILE 3. Fresh Cement, Maximum Ion Content, No Rebar

*INPUT FILE*

```
SOLUTION 1
    temp      15
    pH        7.5
    pe        4
    redox     pe
    units     mmol/kgw
    density   1
    Alkalinity 0
    Cl(-1)    7.5
    Li        1e-010
    Al        1e-010
    Ca        3.1
    Mg        5
    Na        18
    K         1.9
    S(6)      7.3
    N(5)      7.9
    C(4)      21.8
    Br(-1)    0
    Si        0.01
    -water    1 # kg

GAS_PHASE 1
    -fixed_pressure
    -pressure 1
    -volume 1000
    -temperature 25
    CO2(g)    0.056
    O2(g)     0.18
EQUILIBRIUM_PHASES 1
```

```
    Brucite   0 1.39
    Ca(OH)2*(CSH(1.5)) 0 9.5
    Calcite   0 0.001
    CSH(1.0-2.5) 0 15.96
    Gibbsite  0 0.001
    goethite  0 1e-005
    KOH(cement) 0 0.99
    NaOH(cement) 0 0.15
    SiO2(am)  0 0.02
SAVE solution 1-1
END
```

*SAMPLE OUTPUT, INITIAL CONDITION (FILE 3)*

```
 -------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 1.

-----------------------------Solution composition------------------------------

      Elements          Molality       Moles

      Al             1.000e-013  1.000e-013
      C(4)            2.180e-002  2.180e-002
      Ca              3.100e-003  3.100e-003
      Cl(-1)          7.500e-003  7.500e-003
      K              1.900e-003  1.900e-003
      Li             1.000e-013  1.000e-013
      Mg              5.000e-003  5.000e-003
      N(5)            7.900e-003  7.900e-003
      Na              1.800e-002  1.800e-002
      S(6)            7.300e-003  7.300e-003
      Si             1.000e-005  1.000e-005

----------------------------Description of solution----------------------------

                                pH  =   7.500
                                pe  =   4.000
                    Activity of water  =   0.999
                       Ionic strength  =  5.066e-002
                      Mass of water (kg)  =  1.000e+000
                Total alkalinity (eq/kg)  =  2.058e-002
                     Total CO2 (mol/kg)  =  2.180e-002
                    Temperature (deg C)  =  15.000
                  Electrical balance (eq)  = -1.448e-002
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  = -18.54
                           Iterations  =   4
                             Total H  = 1.110710e+002
                             Total O  = 5.564231e+001
```

*SAMPLE OUTPUT, FINAL TIME STEP (FILE 3)*

```
 -------------------------------------------
Beginning of batch-reaction calculations.
-------------------------------------------

Reaction step 1.

Using solution 1.
Using pure phase assemblage 1.
```

Using gas phase 1.

----------Gas phase----------

Total pressure: 1.0000 atmospheres
Gas volume: 1.74e+002 liters

| Component | log P | P | Moles in gas Initial | Final | Delta |
|---|---|---|---|---|---|
| CO2(g) | -12.55 | 2.849e-013 | 2.289e+000 | 2.095e-012 | -2.289e+000 |
| O2(g) | 0.00 | 1.000e+000 | 7.357e+000 | 7.356e+000 | -1.278e-003 |

----------Phase assemblage----------

| Phase | SI | log IAP | log KT | Moles in assemblage Initial | Final | Delta |
|---|---|---|---|---|---|---|
| Brucite | -0.00 | 16.96 | 16.96 | 1.390e+000 | 1.395e+000 | 5.000e-003 |
| Ca(OH)2*(CSH(1.5)) | 0.00 | 22.28 | 22.28 | 9.500e+000 | 7.226e+000 | -2.274e+000 |
| Calcite | -0.00 | 1.98 | 1.98 | 1.000e-003 | 2.295e+000 | 2.294e+000 |
| CSH(1.0-2.5) | 0.00 | 14.80 | 14.80 | 1.596e+001 | 1.594e+001 | -1.696e-002 |
| Gibbsite | -1.67 | 6.69 | 8.36 | 1.000e-003 | 0 | -1.000e-003 |
| Goethite | 0.00 | 0.91 | 0.91 | 1.000e-005 | 9.643e-006 | -3.572e-007 |
| KOH(cement) | -0.73 | 13.73 | 14.46 | 9.900e-001 | 0 | -9.900e-001 |
| NaOH(cement) | -1.12 | 13.06 | 14.18 | 1.500e-001 | 0 | -1.500e-001 |
| SiO2(am) | -4.60 | -7.48 | -2.87 | 2.000e-002 | 0 | -2.000e-002 |

----------Solution composition----------

| Elements | Molality | Moles |
|---|---|---|
| Al | 9.600e-004 | 1.000e-003 |
| C | 1.623e-002 | 1.691e-002 |
| Ca | 4.732e-005 | 4.929e-005 |
| Cl | 7.200e-003 | 7.500e-003 |
| Fe | 3.429e-007 | 3.572e-007 |
| K | 9.522e-001 | 9.919e-001 |
| Li | 9.600e-014 | 1.000e-013 |
| Mg | 3.859e-011 | 4.020e-011 |
| N | 7.584e-003 | 7.900e-003 |
| Na | 1.613e-001 | 1.680e-001 |
| S | 7.008e-003 | 7.300e-003 |
| Si | 3.549e-002 | 3.697e-002 |

----------Description of solution----------

pH = 14.080 Charge balance
pe = 7.455 Adjusted to redox equilibrium
Activity of water = 0.966
Ionic strength = 9.688e-001
Mass of water (kg) = 1.042e+000
Total alkalinity (eq/kg) = 1.102e+000
Total CO2 (mol/kg) = 1.623e-002
Temperature (deg C) = 15.000
Electrical balance (eq) = -1.448e-002
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.76
Iterations = 45
Total H = 1.167855e+002
Total O = 5.912967e+001

----------Distribution of species----------

| Species | Molality | Log Activity | Log Molality | Log Activity | Gamma |
|---|---|---|---|---|---|
| OH- | 8.003e-001 | 5.108e-001 | -0.097 | -0.292 | -0.195 |
| H+ | 1.022e-014 | 8.323e-015 | -13.991 | -14.080 | -0.089 |
| H2O | 5.553e+001 | 9.663e-001 | 1.744 | -0.015 | 0.000 |
| Al | 9.600e-004 | | | | |
| AlO2- | 9.497e-004 | 6.295e-004 | -3.022 | -3.201 | -0.179 |
| NaAlO2 | 1.032e-005 | 1.032e-005 | -4.986 | -4.986 | 0.000 |
| HAlO2 | 2.553e-011 | 2.553e-011 | -10.593 | -10.593 | 0.000 |
| Al(OH)2+ | 4.209e-019 | 2.790e-019 | -18.376 | -18.554 | -0.179 |
| AlOH+2 | 1.210e-026 | 2.044e-027 | -25.917 | -26.689 | -0.772 |
| Al+3 | 4.014e-035 | 3.136e-036 | -34.396 | -35.504 | -1.107 |
| AlSO4+ | 2.577e-036 | 1.708e-036 | -35.589 | -35.767 | -0.179 |
| Al(SO4)2- | 1.065e-037 | 7.058e-038 | -36.973 | -37.151 | -0.179 |
| Al2(OH)2+4 | 0.000e+000 | 0.000e+000 | -47.741 | -50.568 | -2.827 |
| Al3(OH)4+5 | 0.000e+000 | 0.000e+000 | -59.939 | -64.132 | -4.193 |
| Al13O4(OH)24+7 | 0.000e+000 | 0.000e+000 | -101.890 | -110.144 | -8.254 |
| C(-2) | 0.000e+000 | | | | |
| C2H4 | 0.000e+000 | 0.000e+000 | -295.854 | -295.854 | 0.000 |
| C(-3) | 0.000e+000 | | | | |
| C2H6 | 0.000e+000 | 0.000e+000 | -267.719 | -267.719 | 0.000 |
| C(-4) | 0.000e+000 | | | | |
| CH4 | 0.000e+000 | 0.000e+000 | -164.045 | -164.045 | 0.000 |
| C(2) | 0.000e+000 | | | | |
| CO | 0.000e+000 | 0.000e+000 | -62.249 | -62.249 | 0.000 |
| C(4) | 1.623e-002 | | | | |
| CO3-2 | 1.457e-002 | 2.462e-003 | -1.837 | -2.609 | -0.772 |
| NaCO3- | 1.654e-003 | 1.096e-003 | -2.782 | -2.960 | -0.179 |
| CaCO3 | 6.322e-006 | 6.322e-006 | -5.199 | -5.199 | 0.000 |
| HCO3- | 8.595e-007 | 5.697e-007 | -6.066 | -6.244 | -0.179 |
| NaHCO3 | 9.703e-008 | 9.703e-008 | -7.013 | -7.013 | 0.000 |
| MgCO3 | 1.540e-011 | 1.540e-011 | -10.813 | -10.813 | 0.000 |
| CaHCO3+ | 1.410e-011 | 9.344e-012 | -10.851 | -11.029 | -0.179 |
| CO2 | 1.051e-014 | 1.320e-014 | -13.978 | -13.879 | 0.099 |
| MgHCO3+ | 6.657e-017 | 4.413e-017 | -16.177 | -16.355 | -0.179 |
| FeCO3 | 4.363e-034 | 4.363e-034 | -33.360 | -33.360 | 0.000 |
| FeCO3+ | 2.678e-034 | 1.775e-034 | -33.572 | -33.751 | -0.179 |
| FeHCO3+ | 1.141e-039 | 7.566e-040 | -38.943 | -39.121 | -0.179 |
| Ca | 4.732e-005 | | | | |
| CaOH+ | 3.473e-005 | 2.302e-005 | -4.459 | -4.638 | -0.179 |
| CaCO3 | 6.322e-006 | 6.322e-006 | -5.199 | -5.199 | 0.000 |
| Ca+2 | 6.110e-006 | 1.404e-006 | -5.214 | -5.853 | -0.639 |
| CaSO4 | 9.968e-008 | 9.968e-008 | -7.001 | -7.001 | 0.000 |
| CaNO3+ | 4.918e-008 | 3.260e-008 | -7.308 | -7.487 | -0.179 |
| CaCl+ | 1.891e-009 | 1.253e-009 | -8.723 | -8.902 | -0.179 |
| CaHCO3+ | 1.410e-011 | 9.344e-012 | -10.851 | -11.029 | -0.179 |
| CaCl2 | 7.102e-012 | 7.102e-012 | -11.149 | -11.149 | 0.000 |
| Cl(-1) | 7.200e-003 | | | | |
| Cl- | 7.076e-003 | 4.322e-003 | -2.150 | -2.364 | -0.214 |
| NaCl | 6.926e-005 | 6.926e-005 | -4.160 | -4.160 | 0.000 |
| KCl | 5.489e-005 | 5.489e-005 | -4.261 | -4.261 | 0.000 |
| CaCl+ | 1.891e-009 | 1.253e-009 | -8.723 | -8.902 | -0.179 |
| CaCl2 | 7.102e-012 | 7.102e-012 | -11.149 | -11.149 | 0.000 |
| MgCl+ | 3.525e-014 | 2.337e-014 | -13.453 | -13.631 | -0.179 |
| HCl | 7.928e-018 | 7.928e-018 | -17.101 | -17.101 | 0.000 |
| LiCl | 3.156e-018 | 3.156e-018 | -17.501 | -17.501 | 0.000 |
| FeCl+ | 1.155e-038 | 7.657e-039 | -37.937 | -38.116 | -0.179 |
| FeCl2 | 0.000e+000 | 0.000e+000 | -42.773 | -42.773 | 0.000 |

| | | | | | |
|---|---|---|---|---|---|
| FeCl2+ | 0.000e+000 | 0.000e+000 | -43.723 | -43.901 | -0.179 |
| FeCl+2 | 0.000e+000 | 0.000e+000 | -43.896 | -44.668 | -0.772 |
| FeCl4-2 | 0.000e+000 | 0.000e+000 | -46.217 | -47.046 | -0.829 |
| FeCl4- | 0.000e+000 | 0.000e+000 | -51.371 | -51.550 | -0.179 |
| Cl(1) | 7.838e-020 | | | | |
| ClO- | 7.838e-020 | 5.196e-020 | -19.106 | -19.284 | -0.179 |
| HClO | 1.604e-026 | 1.604e-026 | -25.795 | -25.795 | 0.000 |
| Cl(3) | 1.563e-029 | | | | |
| ClO2- | 1.563e-029 | 1.036e-029 | -28.806 | -28.985 | -0.179 |
| HClO2 | 1.275e-040 | 1.275e-040 | -39.894 | -39.894 | 0.000 |
| Cl(5) | 6.930e-025 | | | | |
| ClO3- | 6.930e-025 | 4.423e-025 | -24.159 | -24.354 | -0.195 |
| Cl(7) | 1.241e-024 | | | | |
| ClO4- | 1.241e-024 | 7.920e-025 | -23.906 | -24.101 | -0.195 |
| Fe(2) | 9.077e-025 | | | | |
| Fe(OH)3- | 5.973e-025 | 3.960e-025 | -24.224 | -24.402 | -0.179 |
| Fe(OH)4-2 | 3.102e-025 | 4.597e-026 | -24.508 | -25.338 | -0.829 |
| Fe(OH)2 | 8.567e-029 | 8.567e-029 | -28.067 | -28.067 | 0.000 |
| FeOH+ | 1.402e-031 | 9.290e-032 | -30.853 | -31.032 | -0.179 |
| FeCO3 | 4.363e-034 | 4.363e-034 | -33.360 | -33.360 | 0.000 |
| Fe+2 | 1.101e-035 | 2.531e-036 | -34.958 | -35.597 | -0.639 |
| FeSO4 | 2.135e-037 | 2.135e-037 | -36.671 | -36.671 | 0.000 |
| FeCl+ | 1.155e-038 | 7.657e-039 | -37.937 | -38.116 | -0.179 |
| FeHCO3+ | 1.141e-039 | 7.566e-040 | -38.943 | -39.121 | -0.179 |
| FeCl2 | 0.000e+000 | 0.000e+000 | -42.773 | -42.773 | 0.000 |
| FeCl4-2 | 0.000e+000 | 0.000e+000 | -46.217 | -47.046 | -0.829 |
| Fe(3) | 3.429e-007 | | | | |
| Fe(OH)4- | 3.429e-007 | 2.273e-007 | -6.465 | -6.643 | -0.179 |
| Fe(OH)3 | 7.795e-012 | 7.795e-012 | -11.108 | -11.108 | 0.000 |
| Fe(OH)2+ | 2.166e-019 | 1.435e-019 | -18.664 | -18.843 | -0.179 |
| FeOH+2 | 2.210e-029 | 3.734e-030 | -28.656 | -29.428 | -0.772 |
| FeCO3+ | 2.678e-034 | 1.775e-034 | -33.572 | -33.751 | -0.179 |
| Fe+3 | 0.000e+000 | 0.000e+000 | -40.195 | -41.303 | -1.107 |
| FeNO3+2 | 0.000e+000 | 0.000e+000 | -41.865 | -42.637 | -0.772 |
| FeSO4+ | 0.000e+000 | 0.000e+000 | -42.577 | -42.755 | -0.179 |
| FeCl2+ | 0.000e+000 | 0.000e+000 | -43.723 | -43.901 | -0.179 |
| FeCl+2 | 0.000e+000 | 0.000e+000 | -43.896 | -44.668 | -0.772 |
| Fe(SO4)2- | 0.000e+000 | 0.000e+000 | -44.458 | -44.637 | -0.179 |
| FeCl4- | 0.000e+000 | 0.000e+000 | -51.371 | -51.550 | -0.179 |
| FeNO2+2 | 0.000e+000 | 0.000e+000 | -54.123 | -54.895 | -0.772 |
| Fe2(OH)2+4 | 0.000e+000 | 0.000e+000 | -54.599 | -57.426 | -2.827 |
| Fe3(OH)4+5 | 0.000e+000 | 0.000e+000 | -69.756 | -73.949 | -4.193 |
| H(0) | 0.000e+000 | | | | |
| H2 | 0.000e+000 | 0.000e+000 | -46.477 | -46.378 | 0.099 |
| K | 9.522e-001 | | | | |
| K+ | 7.620e-001 | 4.654e-001 | -0.118 | -0.332 | -0.214 |
| KOH | 1.873e-001 | 1.873e-001 | -0.727 | -0.727 | 0.000 |
| KSO4- | 2.894e-003 | 1.918e-003 | -2.539 | -2.717 | -0.179 |
| KCl | 5.489e-005 | 5.489e-005 | -4.261 | -4.261 | 0.000 |
| KHSO4 | 9.699e-018 | 9.699e-018 | -17.013 | -17.013 | 0.000 |
| Li | 9.600e-014 | | | | |
| LiOH | 6.357e-014 | 6.357e-014 | -13.197 | -13.197 | 0.000 |
| Li+ | 3.231e-014 | 2.390e-014 | -13.491 | -13.622 | -0.131 |
| LiSO4- | 1.130e-016 | 7.493e-017 | -15.947 | -16.125 | -0.179 |
| LiCl | 3.156e-018 | 3.156e-018 | -17.501 | -17.501 | 0.000 |
| Mg | 3.859e-011 | | | | |
| Mg+2 | 2.241e-011 | 6.821e-012 | -10.649 | -11.166 | -0.517 |
| MgCO3 | 1.540e-011 | 1.540e-011 | -10.813 | -10.813 | 0.000 |
| MgSO4 | 7.448e-013 | 7.448e-013 | -12.128 | -12.128 | 0.000 |
| MgCl+ | 3.525e-014 | 2.337e-014 | -13.453 | -13.631 | -0.179 |
| MgHCO3+ | 6.657e-017 | 4.413e-017 | -16.177 | -16.355 | -0.179 |
| Mg4(OH)4+4 | 4.693e-026 | 6.992e-029 | -25.329 | -28.155 | -2.827 |

| | | | | | | |
|---|---|---|---|---|---|---|
| N(-03) | 0.000e+000 | | | | | |
| N3- | 0.000e+000 | 0.000e+000 | -116.375 | -116.553 | -0.179 | |
| HN3 | 0.000e+000 | 0.000e+000 | -125.838 | -125.838 | 0.000 | |
| N(-3) | 0.000e+000 | | | | | |
| NH3 | 0.000e+000 | 0.000e+000 | -75.215 | -75.215 | 0.000 | |
| NH4+ | 0.000e+000 | 0.000e+000 | -79.503 | -79.740 | -0.237 | |
| NH4SO4- | 0.000e+000 | 0.000e+000 | -91.450 | -91.629 | -0.179 | |
| N(0) | 2.136e-034 | | | | | |
| N2 | 1.068e-034 | 1.068e-034 | -33.972 | -33.972 | 0.000 | |
| N(3) | 2.964e-017 | | | | | |
| NO2- | 2.964e-017 | 1.811e-017 | -16.528 | -16.742 | -0.214 | |
| HNO2 | 3.187e-028 | 3.187e-028 | -27.497 | -27.497 | 0.000 | |
| FeNO2+2 | 0.000e+000 | 0.000e+000 | -54.123 | -54.895 | -0.772 | |
| N(5) | 7.584e-003 | | | | | |
| NO3- | 7.584e-003 | 4.632e-003 | -2.120 | -2.334 | -0.214 | |
| CaNO3+ | 4.918e-008 | 3.260e-008 | -7.308 | -7.487 | -0.179 | |
| HNO3 | 1.586e-018 | 1.586e-018 | -17.800 | -17.800 | 0.000 | |
| FeNO3+2 | 0.000e+000 | 0.000e+000 | -41.865 | -42.637 | -0.772 | |
| Na | 1.613e-001 | | | | | |
| Na+ | 1.484e-001 | 9.836e-002 | -0.829 | -1.007 | -0.179 | |
| NaOH | 8.884e-003 | 8.884e-003 | -2.051 | -2.051 | 0.000 | |
| NaHSiO3 | 1.760e-003 | 1.760e-003 | -2.755 | -2.755 | 0.000 | |
| NaCO3- | 1.654e-003 | 1.096e-003 | -2.782 | -2.960 | -0.179 | |
| NaSO4- | 5.219e-004 | 3.459e-004 | -3.282 | -3.461 | -0.179 | |
| NaCl | 6.926e-005 | 6.926e-005 | -4.160 | -4.160 | 0.000 | |
| NaAlO2 | 1.032e-005 | 1.032e-005 | -4.986 | -4.986 | 0.000 | |
| NaHCO3 | 9.703e-008 | 9.703e-008 | -7.013 | -7.013 | 0.000 | |
| O(0) | 2.454e-003 | | | | | |
| O2 | 1.227e-003 | 1.541e-003 | -2.911 | -2.812 | 0.099 | |
| S(-2) | 0.000e+000 | | | | | |
| S-2 | 0.000e+000 | 0.000e+000 | -153.704 | -154.426 | -0.722 | |
| HS- | 0.000e+000 | 0.000e+000 | -155.084 | -155.279 | -0.195 | |
| H2S | 0.000e+000 | 0.000e+000 | -162.208 | -162.208 | 0.000 | |
| S2-2 | 0.000e+000 | 0.000e+000 | -276.543 | -277.372 | -0.829 | |
| S3-2 | 0.000e+000 | 0.000e+000 | -399.526 | -400.355 | -0.829 | |
| S4-2 | 0.000e+000 | 0.000e+000 | -522.740 | -523.569 | -0.829 | |
| S5-2 | 0.000e+000 | 0.000e+000 | -646.180 | -647.009 | -0.829 | |
| S(2) | 0.000e+000 | | | | | |
| S2O3-2 | 0.000e+000 | 0.000e+000 | -166.910 | -167.739 | -0.829 | |
| HS2O3- | 0.000e+000 | 0.000e+000 | -180.626 | -180.805 | -0.179 | |
| S(3) | 0.000e+000 | | | | | |
| S2O4-2 | 0.000e+000 | 0.000e+000 | -152.664 | -153.387 | -0.722 | |
| S(4) | 0.000e+000 | | | | | |
| SO3-2 | 0.000e+000 | 0.000e+000 | -49.342 | -50.114 | -0.772 | |
| HSO3- | 0.000e+000 | 0.000e+000 | -56.836 | -57.015 | -0.179 | |
| H2SO3 | 0.000e+000 | 0.000e+000 | -69.060 | -69.060 | 0.000 | |
| SO2 | 0.000e+000 | 0.000e+000 | -69.298 | -69.298 | 0.000 | |
| S2O6-2 | 0.000e+000 | 0.000e+000 | -85.990 | -86.820 | -0.829 | |
| S3O6-2 | 0.000e+000 | 0.000e+000 | -211.503 | -212.332 | -0.829 | |
| S4O6-2 | 0.000e+000 | 0.000e+000 | -320.749 | -321.578 | -0.829 | |
| S5O6-2 | 0.000e+000 | 0.000e+000 | -459.501 | -460.331 | -0.829 | |
| S(5) | 0.000e+000 | | | | | |
| S2O5-2 | 0.000e+000 | 0.000e+000 | -117.995 | -118.825 | -0.829 | |
| S(6) | 7.008e-003 | | | | | |
| SO4-2 | 3.593e-003 | 5.323e-004 | -2.445 | -3.274 | -0.829 | |
| KSO4- | 2.894e-003 | 1.918e-003 | -2.539 | -2.717 | -0.179 | |
| NaSO4- | 5.219e-004 | 3.459e-004 | -3.282 | -3.461 | -0.179 | |
| CaSO4 | 9.968e-008 | 9.968e-008 | -7.001 | -7.001 | 0.000 | |
| MgSO4 | 7.448e-013 | 7.448e-013 | -12.128 | -12.128 | 0.000 | |
| HSO4- | 5.097e-016 | 3.378e-016 | -15.293 | -15.471 | -0.179 | |
| LiSO4- | 1.130e-016 | 7.493e-017 | -15.947 | -16.125 | -0.179 | |
| KHSO4 | 9.699e-018 | 9.699e-018 | -17.013 | -17.013 | 0.000 | |

```
   H2SO4              3.515e-033  3.515e-033   -32.454   -32.454     0.000
   AlSO4+             2.577e-036  1.708e-036   -35.589   -35.767    -0.179
   FeSO4              2.135e-037  2.135e-037   -36.671   -36.671     0.000
   Al(SO4)2-          1.065e-037  7.058e-038   -36.973   -37.151    -0.179
   FeSO4+             0.000e+000  0.000e+000   -42.577   -42.755    -0.179
   Fe(SO4)2-          0.000e+000  0.000e+000   -44.458   -44.637    -0.179
   NH4SO4-            0.000e+000  0.000e+000   -91.450   -91.629    -0.179
S(7)          0.000e+000
   S2O8-2             0.000e+000  0.000e+000   -58.907   -59.736    -0.829
S(8)          2.037e-037
   HSO5-              2.037e-037  1.350e-037   -36.691   -36.870    -0.179
Si            3.549e-002
   H2SiO4-2           3.325e-002  4.927e-003    -1.478    -2.307    -0.829
   NaHSiO3            1.760e-003  1.760e-003    -2.755    -2.755     0.000
   HSiO3-             4.714e-004  3.125e-004    -3.327    -3.505    -0.179
   H4(H2SiO4)4-4      6.076e-007  2.247e-010    -6.216    -9.648    -3.432
   SiO2               3.334e-008  3.334e-008    -7.477    -7.477     0.000
   H6(H2SiO4)4-2      2.097e-015  3.107e-016   -14.678   -15.508    -0.829
```

## FILE 4. Fresh Cement, Maximum Ion Content, With Rebar

*INPUT FILE*

```
SOLUTION 1
   temp      15
   pH        7.5
   pe        4
   redox     pe
   units     mmol/kgw
   density   1
   Alkalinity 0
   Cl(-1)    7.5
   Li        1e-010
   Al        1e-010
   Ca        3.1
   Mg        5
   Na        18
   K         1.9
   S(6)      7.3
   N(5)      7.9
   C(4)      21.8
   Br(-1)    0
   Si        0.01
   -water    1 # kg

GAS_PHASE 1
   -fixed_pressure
   -pressure 1
   -volume 1000
   -temperature 25
   CO2(g)    0.056
   O2(g)     0.18
EQUILIBRIUM_PHASES 1
   Brucite   0 1.39
   Ca(OH)2*(CSH(1.5)) 0 9.5
   Calcite   0 0.001
   CSH(1.0-2.5) 0 15.96
   Gibbsite  0 0.001
   goethite  0 1e-005
   KOH(cement) 0 0.99
   NaOH(cement) 0 0.15
   SiO2(am)  0 0.02
```

```
REACTION 1
   Fe       1
   4.75 moles in 60 steps
SAVE solution 1-1
END
```

## *SAMPLE OUTPUT, INITIAL CONDITION (FILE 4)*

```
 -----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------

Initial solution 1.

-----------------------------Solution composition------------------------------

      Elements          Molality       Moles

      Al             1.000e-013  1.000e-013
      C(4)            2.180e-002  2.180e-002
      Ca              3.100e-003  3.100e-003
      Cl(-1)          7.500e-003  7.500e-003
      K              1.900e-003  1.900e-003
      Li             1.000e-013  1.000e-013
      Mg              5.000e-003  5.000e-003
      N(5)            7.900e-003  7.900e-003
      Na              1.800e-002  1.800e-002
      S(6)            7.300e-003  7.300e-003
      Si             1.000e-005  1.000e-005

----------------------------Description of solution----------------------------

                                pH  =   7.500
                                pe  =   4.000
                    Activity of water  =   0.999
                       Ionic strength  =  5.066e-002
                    Mass of water (kg)  =  1.000e+000
               Total alkalinity (eq/kg)  =  2.058e-002
                   Total CO2 (mol/kg)  =  2.180e-002
                  Temperature (deg C)  =  15.000
                Electrical balance (eq)  = -1.448e-002
Percent error, 100*(Cat-|An|)/(Cat+|An|)  = -18.54
                          Iterations  =   4
                             Total H  = 1.110710e+002
                             Total O  = 5.564231e+001
```

## *SAMPLE OUTPUT, FINAL TIME STEP (FILE 4)*

```
Reaction step 60.

Using solution 1.
Using pure phase assemblage 1.
Using gas phase 1.
Using reaction 1.

Reaction 1.       Irreversible reaction defined in simulation 1.

      4.750e+000 moles of the following reaction have been added:

                  Relative
      Reactant          moles
```

```
      Fe                1.00000

                  Relative
      Element          moles
      Fe                1.00000

-----------------------------------Gas phase------------------------------------


Total pressure:   1.0000   atmospheres
   Gas volume:  8.97e+001 liters

                                        Moles in gas
                                    ---------------------------------
Component              log P          P     Initial       Final       Delta

CO2(g)                -12.55  2.845e-013  2.289e+000  1.079e-012 -2.289e+000
O2(g)                 -0.00  1.000e+000  7.357e+000  3.793e+000 -3.564e+000

--------------------------------Phase assemblage--------------------------------

                                        Moles in assemblage
Phase                 SI log IAP  log KT      Initial       Final       Delta

Brucite             0.00   16.96   16.96   1.390e+000  1.395e+000  5.000e-003
Ca(OH)2*(CSH(1.5))   0.00   22.28   22.28   9.500e+000  7.228e+000 -2.272e+000
Calcite             0.00    1.98    1.98   1.000e-003  2.294e+000  2.293e+000
CSH(1.0-2.5)         0.00   14.80   14.80   1.596e+001  1.594e+001 -1.815e-002
Gibbsite           -1.67    6.69    8.36   1.000e-003           0 -1.000e-003
Goethite           -0.00    0.91    0.91   1.000e-005  4.750e+000  4.750e+000
KOH(cement)         -0.70   13.76   14.46   9.900e-001           0 -9.900e-001
NaOH(cement)        -1.09   13.09   14.18   1.500e-001           0 -1.500e-001
SiO2(am)            -4.60   -7.48   -2.87   2.000e-002           0 -2.000e-002

------------------------------Solution composition------------------------------

      Elements           Molality       Moles

      Al              1.001e-003  1.000e-003
      C               1.750e-002  1.748e-002
      Ca               4.596e-005  4.591e-005
      Cl              7.508e-003  7.500e-003
      Fe               3.534e-007  3.530e-007
      K               9.930e-001  9.919e-001
      Li              1.001e-013  1.000e-013
      Mg               3.730e-011  3.726e-011
      N               7.909e-003  7.900e-003
      Na               1.682e-001  1.680e-001
      S               7.308e-003  7.300e-003
      Si              3.820e-002  3.816e-002

----------------------------Description of solution----------------------------

                                pH  =  14.094      Charge balance
                                pe  =   7.441      Adjusted to redox equilibrium
                     Activity of water  =   0.965
                        Ionic strength  =  1.007e+000
                     Mass of water (kg)  =  9.989e-001
                Total alkalinity (eq/kg)  =  1.149e+000
                     Total CO2 (mol/kg)  =  1.750e-002
                    Temperature (deg C)  =  15.000
                Electrical balance (eq)  = -1.448e-002
```

Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.76
Iterations = 52
Total H = 1.120343e+002
Total O = 5.675750e+001

----------Distribution of species----------

| Species | Molality | Log Activity | Log Molality | Log Activity | Gamma |
|---|---|---|---|---|---|
| OH- | 8.263e-001 | 5.267e-001 | -0.083 | -0.278 | -0.196 |
| H+ | 9.874e-015 | 8.061e-015 | -14.006 | -14.094 | -0.088 |
| H2O | 5.553e+001 | 9.650e-001 | 1.744 | -0.015 | 0.000 |
| Al | 1.001e-003 | | | | |
| AlO2- | 9.900e-004 | 6.557e-004 | -3.004 | -3.183 | -0.179 |
| NaAlO2 | 1.117e-005 | 1.117e-005 | -4.952 | -4.952 | 0.000 |
| HAlO2 | 2.575e-011 | 2.575e-011 | -10.589 | -10.589 | 0.000 |
| Al(OH)2+ | 4.115e-019 | 2.726e-019 | -18.386 | -18.564 | -0.179 |
| AlOH+2 | 1.159e-026 | 1.937e-027 | -25.936 | -26.713 | -0.777 |
| Al+3 | 3.725e-035 | 2.882e-036 | -34.429 | -35.540 | -1.111 |
| AlSO4+ | 2.412e-036 | 1.598e-036 | -35.618 | -35.796 | -0.179 |
| Al(SO4)2- | 1.015e-037 | 6.721e-038 | -36.994 | -37.173 | -0.179 |
| Al2(OH)2+4 | 0.000e+000 | 0.000e+000 | -47.769 | -50.615 | -2.845 |
| Al3(OH)4+5 | 0.000e+000 | 0.000e+000 | -59.970 | -64.189 | -4.219 |
| Al13O4(OH)24+7 | 0.000e+000 | 0.000e+000 | -101.886 | -110.193 | -8.307 |
| C(-2) | 0.000e+000 | | | | |
| C2H4 | 0.000e+000 | 0.000e+000 | -295.856 | -295.856 | 0.000 |
| C(-3) | 0.000e+000 | | | | |
| C2H6 | 0.000e+000 | 0.000e+000 | -267.722 | -267.722 | 0.000 |
| C(-4) | 0.000e+000 | | | | |
| CH4 | 0.000e+000 | 0.000e+000 | -164.047 | -164.047 | 0.000 |
| C(2) | 0.000e+000 | | | | |
| CO | 0.000e+000 | 0.000e+000 | -62.250 | -62.250 | 0.000 |
| C(4) | 1.750e-002 | | | | |
| CO3-2 | 1.566e-002 | 2.617e-003 | -1.805 | -2.582 | -0.777 |
| NaCO3- | 1.829e-003 | 1.211e-003 | -2.738 | -2.917 | -0.179 |
| CaCO3 | 6.322e-006 | 6.322e-006 | -5.199 | -5.199 | 0.000 |
| HCO3- | 8.856e-007 | 5.866e-007 | -6.053 | -6.232 | -0.179 |
| NaHCO3 | 1.038e-007 | 1.038e-007 | -6.984 | -6.984 | 0.000 |
| MgCO3 | 1.540e-011 | 1.540e-011 | -10.813 | -10.813 | 0.000 |
| CaHCO3+ | 1.366e-011 | 9.050e-012 | -10.864 | -11.043 | -0.179 |
| CO2 | 1.041e-014 | 1.318e-014 | -13.983 | -13.880 | 0.103 |
| MgHCO3+ | 6.452e-017 | 4.274e-017 | -16.190 | -16.369 | -0.179 |
| FeCO3 | 4.360e-034 | 4.360e-034 | -33.361 | -33.361 | 0.000 |
| FeCO3+ | 2.595e-034 | 1.719e-034 | -33.586 | -33.765 | -0.179 |
| FeHCO3+ | 1.106e-039 | 7.323e-040 | -38.956 | -39.135 | -0.179 |
| Ca | 4.596e-005 | | | | |
| CaOH+ | 3.371e-005 | 2.233e-005 | -4.472 | -4.651 | -0.179 |
| CaCO3 | 6.322e-006 | 6.322e-006 | -5.199 | -5.199 | 0.000 |
| Ca+2 | 5.786e-006 | 1.321e-006 | -5.238 | -5.879 | -0.642 |
| CaSO4 | 9.544e-008 | 9.544e-008 | -7.020 | -7.020 | 0.000 |
| CaNO3+ | 4.816e-008 | 3.190e-008 | -7.317 | -7.496 | -0.179 |
| CaCl+ | 1.851e-009 | 1.226e-009 | -8.733 | -8.911 | -0.179 |
| CaHCO3+ | 1.366e-011 | 9.050e-012 | -10.864 | -11.043 | -0.179 |
| CaCl2 | 7.224e-012 | 7.224e-012 | -11.141 | -11.141 | 0.000 |
| Cl(-1) | 7.508e-003 | | | | |
| Cl- | 7.375e-003 | 4.494e-003 | -2.132 | -2.347 | -0.215 |
| NaCl | 7.484e-005 | 7.484e-005 | -4.126 | -4.126 | 0.000 |
| KCl | 5.905e-005 | 5.905e-005 | -4.229 | -4.229 | 0.000 |
| CaCl+ | 1.851e-009 | 1.226e-009 | -8.733 | -8.911 | -0.179 |
| CaCl2 | 7.224e-012 | 7.224e-012 | -11.141 | -11.141 | 0.000 |
| MgCl+ | 3.450e-014 | 2.285e-014 | -13.462 | -13.641 | -0.179 |

| | | | | | |
|---|---|---|---|---|---|
| HCl | 7.985e-018 | 7.985e-018 | -17.098 | -17.098 | 0.000 |
| LiCl | 3.355e-018 | 3.355e-018 | -17.474 | -17.474 | 0.000 |
| FeCl+ | 1.130e-038 | 7.485e-039 | -37.947 | -38.126 | -0.179 |
| FeCl2 | 0.000e+000 | 0.000e+000 | -42.766 | -42.766 | 0.000 |
| FeCl2+ | 0.000e+000 | 0.000e+000 | -43.729 | -43.908 | -0.179 |
| FeCl+2 | 0.000e+000 | 0.000e+000 | -43.915 | -44.692 | -0.777 |
| FeCl4-2 | 0.000e+000 | 0.000e+000 | -46.170 | -47.005 | -0.835 |
| FeCl4- | 0.000e+000 | 0.000e+000 | -51.344 | -51.522 | -0.179 |
| Cl(1) | 8.157e-020 | | | | |
| ClO- | 8.157e-020 | 5.403e-020 | -19.088 | -19.267 | -0.179 |
| HClO | 1.615e-026 | 1.615e-026 | -25.792 | -25.792 | 0.000 |
| Cl(3) | 1.627e-029 | | | | |
| ClO2- | 1.627e-029 | 1.077e-029 | -28.789 | -28.968 | -0.179 |
| HClO2 | 1.284e-040 | 1.284e-040 | -39.891 | -39.891 | 0.000 |
| Cl(5) | 7.217e-025 | | | | |
| ClO3- | 7.217e-025 | 4.600e-025 | -24.142 | -24.337 | -0.196 |
| Cl(7) | 1.292e-024 | | | | |
| ClO4- | 1.292e-024 | 8.236e-025 | -23.889 | -24.084 | -0.196 |
| Fe(2) | 9.501e-025 | | | | |
| Fe(OH)3- | 6.159e-025 | 4.080e-025 | -24.210 | -24.389 | -0.179 |
| Fe(OH)4-2 | 3.340e-025 | 4.884e-026 | -24.476 | -25.311 | -0.835 |
| Fe(OH)2 | 8.561e-029 | 8.561e-029 | -28.067 | -28.067 | 0.000 |
| FeOH+ | 1.359e-031 | 9.004e-032 | -30.867 | -31.046 | -0.179 |
| FeCO3 | 4.360e-034 | 4.360e-034 | -33.361 | -33.361 | 0.000 |
| Fe+2 | 1.042e-035 | 2.379e-036 | -34.982 | -35.624 | -0.642 |
| FeSO4 | 2.043e-037 | 2.043e-037 | -36.690 | -36.690 | 0.000 |
| FeCl+ | 1.130e-038 | 7.485e-039 | -37.947 | -38.126 | -0.179 |
| FeHCO3+ | 1.106e-039 | 7.323e-040 | -38.956 | -39.135 | -0.179 |
| FeCl2 | 0.000e+000 | 0.000e+000 | -42.766 | -42.766 | 0.000 |
| FeCl4-2 | 0.000e+000 | 0.000e+000 | -46.170 | -47.005 | -0.835 |
| Fe(3) | 3.534e-007 | | | | |
| Fe(OH)4- | 3.533e-007 | 2.341e-007 | -6.452 | -6.631 | -0.179 |
| Fe(OH)3 | 7.784e-012 | 7.784e-012 | -11.109 | -11.109 | 0.000 |
| Fe(OH)2+ | 2.099e-019 | 1.390e-019 | -18.678 | -18.857 | -0.179 |
| FeOH+2 | 2.099e-029 | 3.508e-030 | -28.678 | -29.455 | -0.777 |
| FeCO3+ | 2.595e-034 | 1.719e-034 | -33.586 | -33.765 | -0.179 |
| Fe+3 | 0.000e+000 | 0.000e+000 | -40.232 | -41.343 | -1.111 |
| FeNO3+2 | 0.000e+000 | 0.000e+000 | -41.883 | -42.660 | -0.777 |
| FeSO4+ | 0.000e+000 | 0.000e+000 | -42.609 | -42.788 | -0.179 |
| FeCl2+ | 0.000e+000 | 0.000e+000 | -43.729 | -43.908 | -0.179 |
| FeCl+2 | 0.000e+000 | 0.000e+000 | -43.915 | -44.692 | -0.777 |
| Fe(SO4)2- | 0.000e+000 | 0.000e+000 | -44.483 | -44.662 | -0.179 |
| FeCl4- | 0.000e+000 | 0.000e+000 | -51.344 | -51.522 | -0.179 |
| FeNO2+2 | 0.000e+000 | 0.000e+000 | -54.141 | -54.918 | -0.777 |
| Fe2(OH)2+4 | 0.000e+000 | 0.000e+000 | -54.635 | -57.480 | -2.845 |
| Fe3(OH)4+5 | 0.000e+000 | 0.000e+000 | -69.798 | -74.017 | -4.219 |
| H(0) | 0.000e+000 | | | | |
| H2 | 0.000e+000 | 0.000e+000 | -46.481 | -46.379 | 0.103 |
| K | 9.930e-001 | | | | |
| K+ | 7.901e-001 | 4.815e-001 | -0.102 | -0.317 | -0.215 |
| KOH | 1.998e-001 | 1.998e-001 | -0.699 | -0.699 | 0.000 |
| KSO4- | 3.050e-003 | 2.020e-003 | -2.516 | -2.695 | -0.179 |
| KCl | 5.905e-005 | 5.905e-005 | -4.229 | -4.229 | 0.000 |
| KHSO4 | 9.893e-018 | 9.893e-018 | -17.005 | -17.005 | 0.000 |
| Li | 1.001e-013 | | | | |
| LiOH | 6.700e-014 | 6.700e-014 | -13.174 | -13.174 | 0.000 |
| Li+ | 3.300e-014 | 2.443e-014 | -13.482 | -13.612 | -0.131 |
| LiSO4- | 1.177e-016 | 7.795e-017 | -15.929 | -16.108 | -0.179 |
| LiCl | 3.355e-018 | 3.355e-018 | -17.474 | -17.474 | 0.000 |
| Mg | 3.730e-011 | | | | |
| Mg+2 | 2.115e-011 | 6.416e-012 | -10.675 | -11.193 | -0.518 |
| MgCO3 | 1.540e-011 | 1.540e-011 | -10.813 | -10.813 | 0.000 |

| | | | | | |
|---|---|---|---|---|---|
| MgSO4 | 7.131e-013 | 7.131e-013 | -12.147 | -12.147 | 0.000 |
| MgCl+ | 3.450e-014 | 2.285e-014 | -13.462 | -13.641 | -0.179 |
| MgHCO3+ | 6.452e-017 | 4.274e-017 | -16.190 | -16.369 | -0.179 |
| Mg4(OH)4+4 | 4.332e-026 | 6.186e-029 | -25.363 | -28.209 | -2.845 |
| N(-03) | 0.000e+000 | | | | |
| N3- | 0.000e+000 | 0.000e+000 | -116.350 | -116.529 | -0.179 |
| HN3 | 0.000e+000 | 0.000e+000 | -125.828 | -125.828 | 0.000 |
| N(-3) | 0.000e+000 | | | | |
| NH3 | 0.000e+000 | 0.000e+000 | -75.212 | -75.212 | 0.000 |
| NH4+ | 0.000e+000 | 0.000e+000 | -79.513 | -79.751 | -0.238 |
| NH4SO4- | 0.000e+000 | 0.000e+000 | -91.453 | -91.632 | -0.179 |
| N(0) | 2.172e-034 | | | | |
| N2 | 1.086e-034 | 1.086e-034 | -33.964 | -33.964 | 0.000 |
| N(3) | 3.091e-017 | | | | |
| NO2- | 3.091e-017 | 1.884e-017 | -16.510 | -16.725 | -0.215 |
| HNO2 | 3.211e-028 | 3.211e-028 | -27.493 | -27.493 | 0.000 |
| FeNO2+2 | 0.000e+000 | 0.000e+000 | -54.141 | -54.918 | -0.777 |
| N(5) | 7.909e-003 | | | | |
| NO3- | 7.909e-003 | 4.820e-003 | -2.102 | -2.317 | -0.215 |
| CaNO3+ | 4.816e-008 | 3.190e-008 | -7.317 | -7.496 | -0.179 |
| HNO3 | 1.598e-018 | 1.598e-018 | -17.796 | -17.796 | 0.000 |
| FeNO3+2 | 0.000e+000 | 0.000e+000 | -41.883 | -42.660 | -0.777 |
| Na | 1.682e-001 | | | | |
| Na+ | 1.543e-001 | 1.022e-001 | -0.812 | -0.990 | -0.179 |
| NaOH | 9.520e-003 | 9.520e-003 | -2.021 | -2.021 | 0.000 |
| NaHSiO3 | 1.886e-003 | 1.886e-003 | -2.725 | -2.725 | 0.000 |
| NaCO3- | 1.829e-003 | 1.211e-003 | -2.738 | -2.917 | -0.179 |
| NaSO4- | 5.525e-004 | 3.659e-004 | -3.258 | -3.437 | -0.179 |
| NaCl | 7.484e-005 | 7.484e-005 | -4.126 | -4.126 | 0.000 |
| NaAlO2 | 1.117e-005 | 1.117e-005 | -4.952 | -4.952 | 0.000 |
| NaHCO3 | 1.038e-007 | 1.038e-007 | -6.984 | -6.984 | 0.000 |
| O(0) | 2.432e-003 | | | | |
| O2 | 1.216e-003 | 1.541e-003 | -2.915 | -2.812 | 0.103 |
| S(-2) | 0.000e+000 | | | | |
| S-2 | 0.000e+000 | 0.000e+000 | -153.692 | -154.418 | -0.726 |
| HS- | 0.000e+000 | 0.000e+000 | -155.089 | -155.285 | -0.196 |
| H2S | 0.000e+000 | 0.000e+000 | -162.228 | -162.228 | 0.000 |
| S2-2 | 0.000e+000 | 0.000e+000 | -276.549 | -277.384 | -0.835 |
| S3-2 | 0.000e+000 | 0.000e+000 | -399.551 | -400.386 | -0.835 |
| S4-2 | 0.000e+000 | 0.000e+000 | -522.785 | -523.620 | -0.835 |
| S5-2 | 0.000e+000 | 0.000e+000 | -646.244 | -647.079 | -0.835 |
| S(2) | 0.000e+000 | | | | |
| S2O3-2 | 0.000e+000 | 0.000e+000 | -166.916 | -167.751 | -0.835 |
| HS2O3- | 0.000e+000 | 0.000e+000 | -180.652 | -180.830 | -0.179 |
| S(3) | 0.000e+000 | | | | |
| S2O4-2 | 0.000e+000 | 0.000e+000 | -152.672 | -153.398 | -0.726 |
| S(4) | 0.000e+000 | | | | |
| SO3-2 | 0.000e+000 | 0.000e+000 | -49.329 | -50.106 | -0.777 |
| HSO3- | 0.000e+000 | 0.000e+000 | -56.842 | -57.021 | -0.179 |
| H2SO3 | 0.000e+000 | 0.000e+000 | -69.080 | -69.080 | 0.000 |
| SO2 | 0.000e+000 | 0.000e+000 | -69.318 | -69.318 | 0.000 |
| S2O6-2 | 0.000e+000 | 0.000e+000 | -85.996 | -86.831 | -0.835 |
| S3O6-2 | 0.000e+000 | 0.000e+000 | -211.528 | -212.363 | -0.835 |
| S4O6-2 | 0.000e+000 | 0.000e+000 | -320.794 | -321.629 | -0.835 |
| S5O6-2 | 0.000e+000 | 0.000e+000 | -459.566 | -460.401 | -0.835 |
| S(5) | 0.000e+000 | | | | |
| S2O5-2 | 0.000e+000 | 0.000e+000 | -118.001 | -118.836 | -0.835 |
| S(6) | 7.308e-003 | | | | |
| SO4-2 | 3.706e-003 | 5.419e-004 | -2.431 | -3.266 | -0.835 |
| KSO4- | 3.050e-003 | 2.020e-003 | -2.516 | -2.695 | -0.179 |
| NaSO4- | 5.525e-004 | 3.659e-004 | -3.258 | -3.437 | -0.179 |
| CaSO4 | 9.544e-008 | 9.544e-008 | -7.020 | -7.020 | 0.000 |

```
   MgSO4              7.131e-013  7.131e-013   -12.147   -12.147     0.000
   HSO4-              5.028e-016  3.331e-016   -15.299   -15.477    -0.179
   LiSO4-             1.177e-016  7.795e-017   -15.929   -16.108    -0.179
   KHSO4              9.893e-018  9.893e-018   -17.005   -17.005     0.000
   H2SO4              3.356e-033  3.356e-033   -32.474   -32.474     0.000
   AlSO4+             2.412e-036  1.598e-036   -35.618   -35.796    -0.179
   FeSO4              2.043e-037  2.043e-037   -36.690   -36.690     0.000
   Al(SO4)2-          1.015e-037  6.721e-038   -36.994   -37.173    -0.179
   FeSO4+             0.000e+000  0.000e+000   -42.609   -42.788    -0.179
   Fe(SO4)2-          0.000e+000  0.000e+000   -44.483   -44.662    -0.179
   NH4SO4-            0.000e+000  0.000e+000   -91.453   -91.632    -0.179
S(7)          0.000e+000
   S2O8-2             0.000e+000  0.000e+000   -58.913   -59.748    -0.835
S(8)          2.009e-037
   HSO5-              2.009e-037  1.331e-037   -36.697   -36.876    -0.179
Si            3.820e-002
   H2SiO4-2           3.583e-002  5.239e-003    -1.446    -2.281    -0.835
   NaHSiO3            1.886e-003  1.886e-003    -2.725    -2.725     0.000
   HSiO3-             4.864e-004  3.222e-004    -3.313    -3.492    -0.179
   H4(H2SiO4)4-4      7.279e-007  2.526e-010    -6.138    -9.598    -3.460
   SiO2               3.334e-008  3.334e-008    -7.477    -7.477     0.000
   H6(H2SiO4)4-2      2.240e-015  3.276e-016   -14.650   -15.485    -0.835
```

## FILE 5. Mature Cement, Minimum Ion Content, No Rebar

*INPUT FILE*

```
SOLUTION 1
   temp      15
   pH        7.5
   pe        4
   redox     pe
   units     mmol/kgw
   density   1
   Alkalinity 0
   Cl(-1)    0
   Li        1e-010
   Al        1e-010
   Ca        0.6
   Mg        0.3
   Na        1.3
   K         0
   S(6)      0.3
   N(5)      0
   C(4)      1.4
   Br(-1)    0
   Si        0.01
   -water    1 # kg

GAS_PHASE 1
   -fixed_pressure
   -pressure 1
   -volume 1000
   -temperature 25
   CO2(g)    0.056
   O2(g)     0.18
EQUILIBRIUM_PHASES 1
   Brucite   0 1.39
   Ca(OH)2*(CSH(1.5)) 0 9.5
   Calcite   0 0.001
   CSH(1.0-2.5) 0 15.96
   Gibbsite  0 0.001
```

```
    goethite  0 1e-005
    SiO2(am)  0 0.02
SAVE solution 1-1
END
```

## *SAMPLE OUTPUT, INITIAL CONDITION (FILE 5)*

```
 -------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 1.

-----------------------------Solution composition------------------------------

      Elements          Molality       Moles

      Al             1.000e-013  1.000e-013
      C(4)            1.400e-003  1.400e-003
      Ca              6.000e-004  6.000e-004
      Li             1.000e-013  1.000e-013
      Mg              3.000e-004  3.000e-004
      Na              1.300e-003  1.300e-003
      S(6)            3.000e-004  3.000e-004
      Si             1.000e-005  1.000e-005

----------------------------Description of solution----------------------------

                                  pH  =   7.500
                                  pe  =   4.000
                     Activity of water  =   1.000
                        Ionic strength  =  3.581e-003
                     Mass of water (kg)  =  1.000e+000
                Total alkalinity (eq/kg)  =  1.301e-003
                    Total CO2 (mol/kg)  =  1.400e-003
                   Temperature (deg C)  =  15.000
                 Electrical balance (eq)  =  1.199e-003
Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  24.59
                          Iterations  =   4
                             Total H  = 1.110519e+002
                             Total O  = 5.553064e+001
```

## *SAMPLE OUTPUT, FINAL TIME STEP (FILE 5)*

```
 -------------------------------------------
Beginning of batch-reaction calculations.
 -------------------------------------------

Reaction step 1.

Using solution 1.
Using pure phase assemblage 1.
Using gas phase 1.

-----------------------------------Gas phase------------------------------------


Total pressure:   1.0000   atmospheres
   Gas volume:  1.74e+002 liters

                                        Moles in gas
                                    -----------------------------------
```

| Component | log P | P | Initial | Final | Delta |
|---|---|---|---|---|---|
| CO2(g) | -12.53 | 2.947e-013 | 2.289e+000 | 2.168e-012 | -2.289e+000 |
| O2(g) | -0.00 | 1.000e+000 | 7.357e+000 | 7.356e+000 | -1.597e-003 |

----------Phase assemblage----------

| Phase | SI | log IAP | log KT | Moles in assemblage Initial | Final | Delta |
|---|---|---|---|---|---|---|
| Brucite | 0.00 | 16.96 | 16.96 | 1.390e+000 | 1.390e+000 | 3.000e-004 |
| Ca(OH)2*(CSH(1.5)) | 0.00 | 22.28 | 22.28 | 9.500e+000 | 7.183e+000 | -2.317e+000 |
| Calcite | 0.00 | 1.98 | 1.98 | 1.000e-003 | 2.291e+000 | 2.290e+000 |
| CSH(1.0-2.5) | 0.00 | 14.80 | 14.80 | 1.596e+001 | 1.598e+001 | 2.000e-002 |
| Gibbsite | 0.00 | 8.36 | 8.36 | 1.000e-003 | 3.336e-004 | -6.664e-004 |
| Goethite | -0.00 | 0.91 | 0.91 | 1.000e-005 | 9.994e-006 | -5.650e-009 |
| SiO2(am) | -4.60 | -7.48 | -2.87 | 2.000e-002 | 0 | -2.000e-002 |

----------Solution composition----------

| Elements | Molality | Moles |
|---|---|---|
| Al | 6.400e-004 | 6.664e-004 |
| C | 8.046e-006 | 8.378e-006 |
| Ca | 7.132e-003 | 7.426e-003 |
| Fe | 5.426e-009 | 5.650e-009 |
| Li | 9.604e-014 | 1.000e-013 |
| Mg | 2.749e-008 | 2.862e-008 |
| Na | 1.248e-003 | 1.300e-003 |
| S | 2.881e-004 | 3.000e-004 |
| Si | 1.107e-005 | 1.153e-005 |

----------Description of solution----------

pH = 12.369 Charge balance
pe = 9.158 Adjusted to redox equilibrium
Activity of water = 1.000
Ionic strength = 1.948e-002
Mass of water (kg) = 1.041e+000
Total alkalinity (eq/kg) = 1.570e-002
Total CO2 (mol/kg) = 8.046e-006
Temperature (deg C) = 15.000
Electrical balance (eq) = 1.199e-003
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 4.27
Iterations = 69
Total H = 1.156475e+002
Total O = 5.783638e+001

----------Distribution of species----------

| Species | Molality | Log Activity | Log Molality | Log Activity | Gamma |
|---|---|---|---|---|---|
| OH- | 1.180e-002 | 1.028e-002 | -1.928 | -1.988 | -0.060 |
| H+ | 4.790e-013 | 4.278e-013 | -12.320 | -12.369 | -0.049 |
| H2O | 5.553e+001 | 9.996e-001 | 1.744 | -0.000 | 0.000 |
| Al | 6.400e-004 | | | | |
| AlO2- | 6.399e-004 | 5.590e-004 | -3.194 | -3.253 | -0.059 |
| NaAlO2 | 1.013e-007 | 1.013e-007 | -6.994 | -6.994 | 0.000 |
| HAlO2 | 1.165e-009 | 1.165e-009 | -8.934 | -8.934 | 0.000 |
| Al(OH)2+ | 7.492e-016 | 6.544e-016 | -15.125 | -15.184 | -0.059 |
| AlOH+2 | 4.072e-022 | 2.382e-022 | -21.390 | -21.623 | -0.233 |

| | | | | | |
|---|---|---|---|---|---|
| Al+3 | 5.096e-029 | 1.816e-029 | -28.293 | -28.741 | -0.448 |
| AlSO4+ | 2.789e-030 | 2.436e-030 | -29.555 | -29.613 | -0.059 |
| Al(SO4)2- | 2.838e-032 | 2.479e-032 | -31.547 | -31.606 | -0.059 |
| Al2(OH)2+4 | 2.913e-040 | 0.000e+000 | -39.536 | -40.435 | -0.899 |
| Al3(OH)4+5 | 0.000e+000 | 0.000e+000 | -49.248 | -50.629 | -1.380 |
| Al13O4(OH)24+7 | 0.000e+000 | 0.000e+000 | -73.861 | -76.567 | -2.706 |
| C(-2) | 0.000e+000 | | | | |
| C2H4 | 0.000e+000 | 0.000e+000 | -295.795 | -295.795 | 0.000 |
| C(-3) | 0.000e+000 | | | | |
| C2H6 | 0.000e+000 | 0.000e+000 | -267.646 | -267.646 | 0.000 |
| C(-4) | 0.000e+000 | | | | |
| CH4 | 0.000e+000 | 0.000e+000 | -164.001 | -164.001 | 0.000 |
| C(2) | 0.000e+000 | | | | |
| CO | 0.000e+000 | 0.000e+000 | -62.235 | -62.235 | 0.000 |
| C(4) | 8.046e-006 | | | | |
| CaCO3 | 6.322e-006 | 6.322e-006 | -5.199 | -5.199 | 0.000 |
| CO3-2 | 1.704e-006 | 9.972e-007 | -5.768 | -6.001 | -0.233 |
| HCO3- | 1.358e-008 | 1.186e-008 | -7.867 | -7.926 | -0.059 |
| NaCO3- | 5.621e-009 | 4.910e-009 | -8.250 | -8.309 | -0.059 |
| CaHCO3+ | 5.498e-010 | 4.803e-010 | -9.260 | -9.319 | -0.059 |
| NaHCO3 | 2.233e-011 | 2.233e-011 | -10.651 | -10.651 | 0.000 |
| MgCO3 | 1.540e-011 | 1.540e-011 | -10.813 | -10.813 | 0.000 |
| CO2 | 1.359e-014 | 1.366e-014 | -13.867 | -13.865 | 0.002 |
| MgHCO3+ | 2.597e-015 | 2.268e-015 | -14.586 | -14.644 | -0.059 |
| FeCO3+ | 1.045e-032 | 9.124e-033 | -31.981 | -32.040 | -0.059 |
| FeCO3 | 4.438e-034 | 4.438e-034 | -33.353 | -33.353 | 0.000 |
| FeHCO3+ | 4.528e-038 | 3.955e-038 | -37.344 | -37.403 | -0.059 |
| Ca | 7.132e-003 | | | | |
| Ca+2 | 5.755e-003 | 3.466e-003 | -2.240 | -2.460 | -0.220 |
| CaOH+ | 1.310e-003 | 1.144e-003 | -2.883 | -2.942 | -0.059 |
| CaSO4 | 6.061e-005 | 6.061e-005 | -4.217 | -4.217 | 0.000 |
| CaCO3 | 6.322e-006 | 6.322e-006 | -5.199 | -5.199 | 0.000 |
| CaHCO3+ | 5.498e-010 | 4.803e-010 | -9.260 | -9.319 | -0.059 |
| Fe(2) | 9.405e-027 | | | | |
| Fe(OH)3- | 9.280e-027 | 8.106e-027 | -26.032 | -26.091 | -0.059 |
| Fe(OH)2 | 8.714e-029 | 8.714e-029 | -28.060 | -28.060 | 0.000 |
| Fe(OH)4-2 | 3.271e-029 | 1.894e-029 | -28.485 | -28.723 | -0.237 |
| FeOH+ | 5.375e-030 | 4.695e-030 | -29.270 | -29.328 | -0.059 |
| Fe+2 | 1.055e-032 | 6.354e-033 | -31.977 | -32.197 | -0.220 |
| FeCO3 | 4.438e-034 | 4.438e-034 | -33.353 | -33.353 | 0.000 |
| FeSO4 | 1.320e-034 | 1.320e-034 | -33.879 | -33.879 | 0.000 |
| FeHCO3+ | 4.528e-038 | 3.955e-038 | -37.344 | -37.403 | -0.059 |
| Fe(3) | 5.426e-009 | | | | |
| Fe(OH)4- | 5.418e-009 | 4.733e-009 | -8.266 | -8.325 | -0.059 |
| Fe(OH)3 | 8.064e-012 | 8.064e-012 | -11.093 | -11.093 | 0.000 |
| Fe(OH)2+ | 8.447e-018 | 7.378e-018 | -17.073 | -17.132 | -0.059 |
| FeOH+2 | 1.630e-026 | 9.536e-027 | -25.788 | -26.021 | -0.233 |
| FeCO3+ | 1.045e-032 | 9.124e-033 | -31.981 | -32.040 | -0.059 |
| Fe+3 | 1.774e-036 | 6.321e-037 | -35.751 | -36.199 | -0.448 |
| FeSO4+ | 6.283e-039 | 5.488e-039 | -38.202 | -38.261 | -0.059 |
| Fe(SO4)2- | 0.000e+000 | 0.000e+000 | -40.692 | -40.750 | -0.059 |
| Fe2(OH)2+4 | 0.000e+000 | 0.000e+000 | -49.712 | -50.611 | -0.899 |
| Fe3(OH)4+5 | 0.000e+000 | 0.000e+000 | -64.043 | -65.423 | -1.380 |
| H(0) | 0.000e+000 | | | | |
| H2 | 0.000e+000 | 0.000e+000 | -46.365 | -46.363 | 0.002 |
| Li | 9.604e-014 | | | | |
| Li+ | 9.164e-014 | 8.084e-014 | -13.038 | -13.092 | -0.054 |
| LiOH | 4.327e-015 | 4.327e-015 | -14.364 | -14.364 | 0.000 |
| LiSO4- | 7.145e-017 | 6.241e-017 | -16.146 | -16.205 | -0.059 |
| Mg | 2.749e-008 | | | | |
| Mg+2 | 2.702e-008 | 1.684e-008 | -7.568 | -7.774 | -0.205 |
| MgSO4 | 4.529e-010 | 4.529e-010 | -9.344 | -9.344 | 0.000 |

| | | | | | |
|---|---|---|---|---|---|
| MgCO3 | 1.540e-011 | 1.540e-011 | -10.813 | -10.813 | 0.000 |
| MgHCO3+ | 2.597e-015 | 2.268e-015 | -14.586 | -14.644 | -0.059 |
| Mg4(OH)4+4 | 3.379e-021 | 4.261e-022 | -20.471 | -21.371 | -0.899 |
| Na | 1.248e-003 | | | | |
| Na+ | 1.245e-003 | 1.087e-003 | -2.905 | -2.964 | -0.059 |
| NaOH | 1.977e-006 | 1.977e-006 | -5.704 | -5.704 | 0.000 |
| NaSO4- | 1.078e-006 | 9.420e-007 | -5.967 | -6.026 | -0.059 |
| NaHSiO3 | 3.916e-007 | 3.916e-007 | -6.407 | -6.407 | 0.000 |
| NaAlO2 | 1.013e-007 | 1.013e-007 | -6.994 | -6.994 | 0.000 |
| NaCO3- | 5.621e-009 | 4.910e-009 | -8.250 | -8.309 | -0.059 |
| NaHCO3 | 2.233e-011 | 2.233e-011 | -10.651 | -10.651 | 0.000 |
| O(0) | 3.067e-003 | | | | |
| O2 | 1.533e-003 | 1.541e-003 | -2.814 | -2.812 | 0.002 |
| S(-2) | 0.000e+000 | | | | |
| HS- | 0.000e+000 | 0.000e+000 | -154.117 | -154.176 | -0.060 |
| S-2 | 0.000e+000 | 0.000e+000 | -154.806 | -155.034 | -0.228 |
| H2S | 0.000e+000 | 0.000e+000 | -159.394 | -159.394 | 0.000 |
| S2-2 | 0.000e+000 | 0.000e+000 | -274.945 | -275.182 | -0.237 |
| S3-2 | 0.000e+000 | 0.000e+000 | -395.129 | -395.366 | -0.237 |
| S4-2 | 0.000e+000 | 0.000e+000 | -515.544 | -515.782 | -0.237 |
| S5-2 | 0.000e+000 | 0.000e+000 | -636.186 | -636.423 | -0.237 |
| S(2) | 0.000e+000 | | | | |
| S2O3-2 | 0.000e+000 | 0.000e+000 | -165.312 | -165.549 | -0.237 |
| HS2O3- | 0.000e+000 | 0.000e+000 | -176.845 | -176.904 | -0.059 |
| S(3) | 0.000e+000 | | | | |
| S2O4-2 | 0.000e+000 | 0.000e+000 | -150.968 | -151.196 | -0.228 |
| S(4) | 0.000e+000 | | | | |
| SO3-2 | 0.000e+000 | 0.000e+000 | -50.489 | -50.722 | -0.233 |
| HSO3- | 0.000e+000 | 0.000e+000 | -55.854 | -55.913 | -0.059 |
| H2SO3 | 0.000e+000 | 0.000e+000 | -66.247 | -66.247 | 0.000 |
| SO2 | 0.000e+000 | 0.000e+000 | -66.500 | -66.500 | 0.000 |
| S2O6-2 | 0.000e+000 | 0.000e+000 | -84.392 | -84.630 | -0.237 |
| S3O6-2 | 0.000e+000 | 0.000e+000 | -207.106 | -207.343 | -0.237 |
| S4O6-2 | 0.000e+000 | 0.000e+000 | -313.554 | -313.791 | -0.237 |
| S5O6-2 | 0.000e+000 | 0.000e+000 | -449.507 | -449.745 | -0.237 |
| S(5) | 0.000e+000 | | | | |
| S2O5-2 | 0.000e+000 | 0.000e+000 | -116.397 | -116.635 | -0.237 |
| S(6) | 2.881e-004 | | | | |
| SO4-2 | 2.264e-004 | 1.311e-004 | -3.645 | -3.882 | -0.237 |
| CaSO4 | 6.061e-005 | 6.061e-005 | -4.217 | -4.217 | 0.000 |
| NaSO4- | 1.078e-006 | 9.420e-007 | -5.967 | -6.026 | -0.059 |
| MgSO4 | 4.529e-010 | 4.529e-010 | -9.344 | -9.344 | 0.000 |
| HSO4- | 4.896e-015 | 4.277e-015 | -14.310 | -14.369 | -0.059 |
| LiSO4- | 7.145e-017 | 6.241e-017 | -16.146 | -16.205 | -0.059 |
| AlSO4+ | 2.789e-030 | 2.436e-030 | -29.555 | -29.613 | -0.059 |
| H2SO4 | 2.287e-030 | 2.287e-030 | -29.641 | -29.641 | 0.000 |
| Al(SO4)2- | 2.838e-032 | 2.479e-032 | -31.547 | -31.606 | -0.059 |
| FeSO4 | 1.320e-034 | 1.320e-034 | -33.879 | -33.879 | 0.000 |
| FeSO4+ | 6.283e-039 | 5.488e-039 | -38.202 | -38.261 | -0.059 |
| Fe(SO4)2- | 0.000e+000 | 0.000e+000 | -40.692 | -40.750 | -0.059 |
| S(7) | 0.000e+000 | | | | |
| S2O8-2 | 0.000e+000 | 0.000e+000 | -57.309 | -57.546 | -0.237 |
| S(8) | 1.957e-036 | | | | |
| HSO5- | 1.957e-036 | 1.709e-036 | -35.708 | -35.767 | -0.059 |
| Si | 1.107e-005 | | | | |
| HSiO3- | 7.200e-006 | 6.289e-006 | -5.143 | -5.201 | -0.059 |
| H2SiO4-2 | 3.447e-006 | 1.996e-006 | -5.463 | -5.700 | -0.237 |
| NaHSiO3 | 3.916e-007 | 3.916e-007 | -6.407 | -6.407 | 0.000 |
| SiO2 | 3.334e-008 | 3.334e-008 | -7.477 | -7.477 | 0.000 |
| H4(H2SiO4)4-4 | 3.777e-016 | 4.224e-017 | -15.423 | -16.374 | -0.951 |
| H6(H2SiO4)4-2 | 2.664e-019 | 1.542e-019 | -18.575 | -18.812 | -0.237 |

## File 6. Mature Cement, Minimum Ion Content, With Rebar

*INPUT FILE*

```
SOLUTION 1
   temp      15
   pH        7.5
   pe        4
   redox     pe
   units     mmol/kgw
   density   1
   Alkalinity 0
   Cl(-1)    0
   Li        1e-010
   Al        1e-010
   Ca        0.6
   Mg        0.3
   Na        1.3
   K         0
   S(6)      0.3
   N(5)      0
   C(4)      1.4
   Br(-1)    0
   Si        0.01
   -water    1 # kg

GAS_PHASE 1
   -fixed_pressure
   -pressure 1
   -volume 1000
   -temperature 25
   CO2(g)    0.056
   O2(g)     0.18
EQUILIBRIUM_PHASES 1
   Brucite   0 1.39
   Ca(OH)2*(CSH(1.5)) 0 9.5
   Calcite   0 0.001
   CSH(1.0-2.5) 0 15.96
   Gibbsite  0 0.001
   goethite  0 1e-005
   SiO2(am)  0 0.02
REACTION 1
   Fe        1
   4.75 moles in 60 steps
SAVE solution 1-1
END
```

*SAMPLE OUTPUT, INITIAL CONDITION (FILE 6)*

```
 -------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 1.

-----------------------------Solution composition------------------------------

      Elements           Molality       Moles

      Al              1.000e-013  1.000e-013
      C(4)             2.180e-002  2.180e-002
      Ca               3.100e-003  3.100e-003
      Cl(-1)           7.500e-003  7.500e-003
```

```
K              1.900e-003  1.900e-003
Li             1.000e-013  1.000e-013
Mg             5.000e-003  5.000e-003
N(5)           7.900e-003  7.900e-003
Na             1.800e-002  1.800e-002
S(6)           7.300e-003  7.300e-003
Si             1.000e-005  1.000e-005

----------------------------Description of solution----------------------------

                                    pH  =   7.500
                                    pe  =   4.000
                      Activity of water  =   0.999
                         Ionic strength  =  5.066e-002
                        Mass of water (kg)  =  1.000e+000
                 Total alkalinity (eq/kg)  =  2.058e-002
                      Total CO2 (mol/kg)  =  2.180e-002
                     Temperature (deg C)  =  15.000
                   Electrical balance (eq)  = -1.448e-002
Percent error, 100*(Cat-|An|)/(Cat+|An|)  = -18.54
                              Iterations  =   4
                                 Total H  = 1.110710e+002
                                 Total O  = 5.564231e+001
```

## *SAMPLE OUTPUT, FINAL TIME STEP (FILE 6)*

```
Reaction step 60.

Using solution 1.
Using pure phase assemblage 1.
Using gas phase 1.
Using reaction 1.

Reaction 1.       Irreversible reaction defined in simulation 1.

      4.750e+000 moles of the following reaction have been added:

                  Relative
     Reactant        moles

     Fe             1.00000

                  Relative
     Element         moles
     Fe             1.00000

-----------------------------------Gas phase-----------------------------------


Total pressure:   1.0000   atmospheres
   Gas volume:  8.97e+001 liters

                                        Moles in gas
                                  -----------------------------------
Component             log P          P    Initial      Final       Delta

CO2(g)              -12.53  2.945e-013  2.289e+000  1.117e-012 -2.289e+000
O2(g)                 0.00  1.000e+000  7.357e+000  3.793e+000 -3.564e+000

--------------------------------Phase assemblage--------------------------------

                                        Moles in assemblage
```

| Phase | SI | log IAP | log KT | Initial | Final | Delta |
|---|---|---|---|---|---|---|
| Brucite | 0.00 | 16.96 | 16.96 | 1.390e+000 | 1.395e+000 | 5.000e-003 |
| Ca(OH)2*(CSH(1.5)) | 0.00 | 22.28 | 22.28 | 9.500e+000 | 7.166e+000 | -2.334e+000 |
| Calcite | 0.00 | 1.98 | 1.98 | 1.000e-003 | 2.312e+000 | 2.311e+000 |
| CSH(1.0-2.5) | 0.00 | 14.80 | 14.80 | 1.596e+001 | 1.598e+001 | 1.999e-002 |
| Gibbsite | 0.00 | 8.36 | 8.36 | 1.000e-003 | 1.571e-004 | -8.429e-004 |
| Goethite | -0.00 | 0.91 | 0.91 | 1.000e-005 | 4.750e+000 | 4.750e+000 |
| SiO2(am) | -4.60 | -7.48 | -2.87 | 2.000e-002 | 0 | -2.000e-002 |

----------Solution composition----------

| Elements | Molality | Moles |
|---|---|---|
| Al | 8.438e-004 | 8.429e-004 |
| C | 9.756e-006 | 9.745e-006 |
| Ca | 6.616e-003 | 6.608e-003 |
| Cl | 7.508e-003 | 7.500e-003 |
| Fe | 7.123e-009 | 7.115e-009 |
| K | 1.902e-003 | 1.900e-003 |
| Li | 1.001e-013 | 1.000e-013 |
| Mg | 2.711e-008 | 2.708e-008 |
| N | 7.909e-003 | 7.900e-003 |
| Na | 1.802e-002 | 1.800e-002 |
| S | 7.308e-003 | 7.300e-003 |
| Si | 2.272e-005 | 2.270e-005 |

----------Description of solution----------

pH = 12.463 Charge balance
pe = 9.065 Adjusted to redox equilibrium
Activity of water = 0.999
Ionic strength = 4.775e-002
Mass of water (kg) = 9.989e-001
Total alkalinity (eq/kg) = 2.015e-002
Total CO2 (mol/kg) = 9.756e-006
Temperature (deg C) = 15.000
Electrical balance (eq) = -1.448e-002
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -19.55
Iterations = 74
Total H = 1.109419e+002
Total O = 5.553702e+001

----------Distribution of species----------

| Species | Molality | Log Activity | Log Molality | Log Activity | Gamma |
|---|---|---|---|---|---|
| OH- | 1.555e-002 | 1.275e-002 | -1.808 | -1.894 | -0.086 |
| H+ | 4.004e-013 | 3.446e-013 | -12.397 | -12.463 | -0.065 |
| H2O | 5.553e+001 | 9.989e-001 | 1.744 | -0.000 | 0.000 |
| Al | 8.438e-004 | | | | |
| AlO2- | 8.421e-004 | 6.944e-004 | -3.075 | -3.158 | -0.084 |
| NaAlO2 | 1.683e-006 | 1.683e-006 | -5.774 | -5.774 | 0.000 |
| HAlO2 | 1.166e-009 | 1.166e-009 | -8.933 | -8.933 | 0.000 |
| Al(OH)2+ | 6.399e-016 | 5.276e-016 | -15.194 | -15.278 | -0.084 |
| AlOH+2 | 3.323e-022 | 1.548e-022 | -21.478 | -21.810 | -0.332 |
| Al+3 | 3.801e-029 | 9.514e-030 | -28.420 | -29.022 | -0.602 |
| AlSO4+ | 3.289e-029 | 2.712e-029 | -28.483 | -28.567 | -0.084 |
| Al(SO4)2- | 7.113e-030 | 5.865e-030 | -29.148 | -29.232 | -0.084 |
| Al2(OH)2+4 | 2.848e-040 | 0.000e+000 | -39.546 | -40.809 | -1.264 |
| Al3(OH)4+5 | 0.000e+000 | 0.000e+000 | -49.171 | -51.097 | -1.926 |

| | | | | | | |
|---|---|---|---|---|---|---|
| Al13O4(OH)24+7 | 0.000e+000 | 0.000e+000 | -73.444 | -77.221 | -3.777 | |
| C(-2) | 0.000e+000 | | | | | |
| C2H4 | 0.000e+000 | 0.000e+000 | -295.796 | -295.796 | 0.000 | |
| C(-3) | 0.000e+000 | | | | | |
| C2H6 | 0.000e+000 | 0.000e+000 | -267.647 | -267.647 | 0.000 | |
| C(-4) | 0.000e+000 | | | | | |
| CH4 | 0.000e+000 | 0.000e+000 | -164.002 | -164.002 | 0.000 | |
| C(2) | 0.000e+000 | | | | | |
| CO | 0.000e+000 | 0.000e+000 | -62.235 | -62.235 | 0.000 | |
| C(4) | 9.756e-006 | | | | | |
| CaCO3 | 6.322e-006 | 6.322e-006 | -5.199 | -5.199 | 0.000 | |
| CO3-2 | 3.293e-006 | 1.534e-006 | -5.482 | -5.814 | -0.332 | |
| NaCO3- | 1.225e-007 | 1.010e-007 | -6.912 | -6.996 | -0.084 | |
| HCO3- | 1.783e-008 | 1.470e-008 | -7.749 | -7.833 | -0.084 | |
| CaHCO3+ | 4.693e-010 | 3.869e-010 | -9.329 | -9.412 | -0.084 | |
| NaHCO3 | 3.703e-010 | 3.703e-010 | -9.431 | -9.431 | 0.000 | |
| MgCO3 | 1.540e-011 | 1.540e-011 | -10.813 | -10.813 | 0.000 | |
| CO2 | 1.349e-014 | 1.365e-014 | -13.870 | -13.865 | 0.005 | |
| MgHCO3+ | 2.216e-015 | 1.827e-015 | -14.654 | -14.738 | -0.084 | |
| FeCO3+ | 8.915e-033 | 7.350e-033 | -32.050 | -32.134 | -0.084 | |
| FeCO3 | 4.436e-034 | 4.436e-034 | -33.353 | -33.353 | 0.000 | |
| FeHCO3+ | 3.863e-038 | 3.185e-038 | -37.413 | -37.497 | -0.084 | |
| Ca | 6.616e-003 | | | | | |
| Ca+2 | 4.563e-003 | 2.253e-003 | -2.341 | -2.647 | -0.307 | |
| CaOH+ | 1.119e-003 | 9.223e-004 | -2.951 | -3.035 | -0.084 | |
| CaSO4 | 8.370e-004 | 8.370e-004 | -3.077 | -3.077 | 0.000 | |
| CaNO3+ | 8.729e-005 | 7.197e-005 | -4.059 | -4.143 | -0.084 | |
| CaCO3 | 6.322e-006 | 6.322e-006 | -5.199 | -5.199 | 0.000 | |
| CaCl+ | 3.445e-006 | 2.841e-006 | -5.463 | -5.547 | -0.084 | |
| CaCl2 | 2.273e-008 | 2.273e-008 | -7.643 | -7.643 | 0.000 | |
| CaHCO3+ | 4.693e-010 | 3.869e-010 | -9.329 | -9.412 | -0.084 | |
| Cl(-1) | 7.508e-003 | | | | | |
| Cl- | 7.490e-003 | 6.104e-003 | -2.126 | -2.214 | -0.089 | |
| NaCl | 1.446e-005 | 1.446e-005 | -4.840 | -4.840 | 0.000 | |
| CaCl+ | 3.445e-006 | 2.841e-006 | -5.463 | -5.547 | -0.084 | |
| KCl | 2.508e-007 | 2.508e-007 | -6.601 | -6.601 | 0.000 | |
| CaCl2 | 2.273e-008 | 2.273e-008 | -7.643 | -7.643 | 0.000 | |
| MgCl+ | 6.422e-011 | 5.295e-011 | -10.192 | -10.276 | -0.084 | |
| HCl | 4.637e-016 | 4.637e-016 | -15.334 | -15.334 | 0.000 | |
| LiCl | 1.464e-017 | 1.464e-017 | -16.835 | -16.835 | 0.000 | |
| FeCl+ | 2.140e-035 | 1.764e-035 | -34.670 | -34.753 | -0.084 | |
| FeCl2+ | 2.018e-039 | 1.664e-039 | -38.695 | -38.779 | -0.084 | |
| FeCl2 | 5.493e-040 | 5.493e-040 | -39.260 | -39.260 | 0.000 | |
| FeCl+2 | 4.323e-040 | 2.014e-040 | -39.364 | -39.696 | -0.332 | |
| FeCl4-2 | 0.000e+000 | 0.000e+000 | -42.893 | -43.234 | -0.341 | |
| FeCl4- | 0.000e+000 | 0.000e+000 | -46.044 | -46.128 | -0.084 | |
| Cl(1) | 8.901e-020 | | | | | |
| ClO- | 8.901e-020 | 7.339e-020 | -19.051 | -19.134 | -0.084 | |
| HClO | 9.379e-025 | 9.379e-025 | -24.028 | -24.028 | 0.000 | |
| Cl(3) | 1.775e-029 | | | | | |
| ClO2- | 1.775e-029 | 1.463e-029 | -28.751 | -28.835 | -0.084 | |
| HClO2 | 7.457e-039 | 7.457e-039 | -38.127 | -38.127 | 0.000 | |
| Cl(5) | 7.620e-025 | | | | | |
| ClO3- | 7.620e-025 | 6.248e-025 | -24.118 | -24.204 | -0.086 | |
| Cl(7) | 1.364e-024 | | | | | |
| ClO4- | 1.364e-024 | 1.119e-024 | -23.865 | -23.951 | -0.086 | |
| Fe(2) | 1.235e-026 | | | | | |
| Fe(OH)3- | 1.219e-026 | 1.005e-026 | -25.914 | -25.998 | -0.084 | |
| Fe(OH)2 | 8.711e-029 | 8.711e-029 | -28.060 | -28.060 | 0.000 | |
| Fe(OH)4-2 | 6.386e-029 | 2.913e-029 | -28.195 | -28.536 | -0.341 | |
| FeOH+ | 4.589e-030 | 3.784e-030 | -29.338 | -29.422 | -0.084 | |
| Fe+2 | 8.362e-033 | 4.128e-033 | -32.078 | -32.384 | -0.307 | |

```
  FeSO4              1.823e-033  1.823e-033   -32.739   -32.739     0.000
  FeCO3              4.436e-034  4.436e-034   -33.353   -33.353     0.000
  FeCl+              2.140e-035  1.764e-035   -34.670   -34.753    -0.084
  FeHCO3+            3.863e-038  3.185e-038   -37.413   -37.497    -0.084
  FeCl2              5.493e-040  5.493e-040   -39.260   -39.260     0.000
  FeCl4-2            0.000e+000  0.000e+000   -42.893   -43.234    -0.341
Fe(3)         7.123e-009
  Fe(OH)4-           7.115e-009  5.866e-009    -8.148    -8.232    -0.084
  Fe(OH)3            8.058e-012  8.058e-012   -11.094   -11.094     0.000
  Fe(OH)2+           7.209e-018  5.944e-018   -17.142   -17.226    -0.084
  FeOH+2             1.329e-026  6.193e-027   -25.876   -26.208    -0.332
  FeCO3+             8.915e-033  7.350e-033   -32.050   -32.134    -0.084
  Fe+3               1.322e-036  3.310e-037   -35.879   -36.480    -0.602
  FeSO4+             7.405e-038  6.105e-038   -37.130   -37.214    -0.084
  FeNO3+2            4.527e-038  2.110e-038   -37.344   -37.676    -0.332
  Fe(SO4)2-          5.095e-039  4.201e-039   -38.293   -38.377    -0.084
  FeCl2+             2.018e-039  1.664e-039   -38.695   -38.779    -0.084
  FeCl+2             4.323e-040  2.014e-040   -39.364   -39.696    -0.332
  FeCl4-             0.000e+000  0.000e+000   -46.044   -46.128    -0.084
  FeNO2+2            0.000e+000  0.000e+000   -49.602   -49.934    -0.332
  Fe2(OH)2+4         0.000e+000  0.000e+000   -49.723   -50.986    -1.264
  Fe3(OH)4+5         0.000e+000  0.000e+000   -63.966   -65.892    -1.926
H(0)          0.000e+000
  H2                 0.000e+000  0.000e+000   -46.369   -46.364     0.005
K             1.902e-003
  K+                 1.847e-003  1.506e-003    -2.733    -2.822    -0.089
  KSO4-              3.939e-005  3.247e-005    -4.405    -4.488    -0.084
  KOH                1.513e-005  1.513e-005    -4.820    -4.820     0.000
  KCl                2.508e-007  2.508e-007    -6.601    -6.601     0.000
  KHSO4              6.799e-018  6.799e-018   -17.168   -17.168     0.000
Li            1.001e-013
  Li+                9.333e-014  7.848e-014   -13.030   -13.105    -0.075
  LiOH               5.211e-015  5.211e-015   -14.283   -14.283     0.000
  LiSO4-             1.561e-015  1.287e-015   -14.806   -14.890    -0.084
  LiCl               1.464e-017  1.464e-017   -16.835   -16.835     0.000
Mg            2.711e-008
  Mg+2               2.078e-008  1.094e-008    -7.682    -7.961    -0.279
  MgSO4              6.254e-009  6.254e-009    -8.204    -8.204     0.000
  MgCl+              6.422e-011  5.295e-011   -10.192   -10.276    -0.084
  MgCO3              1.540e-011  1.540e-011   -10.813   -10.813     0.000
  MgHCO3+            2.216e-015  1.827e-015   -14.654   -14.738    -0.084
  Mg4(OH)4+4         3.303e-021  1.800e-022   -20.481   -21.745    -1.264
N(-03)        0.000e+000
  N3-                0.000e+000  0.000e+000  -112.834  -112.918    -0.084
  HN3                0.000e+000  0.000e+000  -120.585  -120.585     0.000
N(-3)         0.000e+000
  NH3                0.000e+000  0.000e+000   -73.445   -73.445     0.000
  NH4+               0.000e+000  0.000e+000   -76.261   -76.353    -0.092
  NH4SO4-            0.000e+000  0.000e+000   -87.439   -87.523    -0.084
N(0)          6.707e-031
  N2                 3.353e-031  3.353e-031   -30.475   -30.475     0.000
N(3)          3.057e-017
  NO2-               3.057e-017  2.491e-017   -16.515   -16.604    -0.089
  HNO2               1.816e-026  1.816e-026   -25.741   -25.741     0.000
  FeNO2+2            0.000e+000  0.000e+000   -49.602   -49.934    -0.332
N(5)          7.909e-003
  NO3-               7.822e-003  6.374e-003    -2.107    -2.196    -0.089
  CaNO3+             8.729e-005  7.197e-005    -4.059    -4.143    -0.084
  HNO3               9.037e-017  9.037e-017   -16.044   -16.044     0.000
  FeNO3+2            4.527e-038  2.110e-038   -37.344   -37.676    -0.332
Na            1.802e-002
  Na+                1.764e-002  1.454e-002    -1.753    -1.837    -0.084
```

| | | | | | |
|---|---|---|---|---|---|
| NaSO4- | 3.247e-004 | 2.677e-004 | -3.489 | -3.572 | -0.084 |
| NaOH | 3.280e-005 | 3.280e-005 | -4.484 | -4.484 | 0.000 |
| NaCl | 1.446e-005 | 1.446e-005 | -4.840 | -4.840 | 0.000 |
| NaHSiO3 | 6.497e-006 | 6.497e-006 | -5.187 | -5.187 | 0.000 |
| NaAlO2 | 1.683e-006 | 1.683e-006 | -5.774 | -5.774 | 0.000 |
| NaCO3- | 1.225e-007 | 1.010e-007 | -6.912 | -6.996 | -0.084 |
| NaHCO3 | 3.703e-010 | 3.703e-010 | -9.431 | -9.431 | 0.000 |
| O(0) | 3.046e-003 | | | | |
| O2 | 1.523e-003 | 1.541e-003 | -2.817 | -2.812 | 0.005 |
| S(-2) | 0.000e+000 | | | | |
| HS- | 0.000e+000 | 0.000e+000 | -152.857 | -152.943 | -0.086 |
| S-2 | 0.000e+000 | 0.000e+000 | -153.384 | -153.707 | -0.323 |
| H2S | 0.000e+000 | 0.000e+000 | -158.255 | -158.255 | 0.000 |
| S2-2 | 0.000e+000 | 0.000e+000 | -272.374 | -272.715 | -0.341 |
| S3-2 | 0.000e+000 | 0.000e+000 | -391.418 | -391.759 | -0.341 |
| S4-2 | 0.000e+000 | 0.000e+000 | -510.694 | -511.035 | -0.341 |
| S5-2 | 0.000e+000 | 0.000e+000 | -630.196 | -630.536 | -0.341 |
| S(2) | 0.000e+000 | | | | |
| S2O3-2 | 0.000e+000 | 0.000e+000 | -162.741 | -163.082 | -0.341 |
| HS2O3- | 0.000e+000 | 0.000e+000 | -174.447 | -174.530 | -0.084 |
| S(3) | 0.000e+000 | | | | |
| S2O4-2 | 0.000e+000 | 0.000e+000 | -148.406 | -148.729 | -0.323 |
| S(4) | 0.000e+000 | | | | |
| SO3-2 | 0.000e+000 | 0.000e+000 | -49.063 | -49.395 | -0.332 |
| HSO3- | 0.000e+000 | 0.000e+000 | -54.595 | -54.679 | -0.084 |
| H2SO3 | 0.000e+000 | 0.000e+000 | -65.107 | -65.107 | 0.000 |
| SO2 | 0.000e+000 | 0.000e+000 | -65.360 | -65.360 | 0.000 |
| S2O6-2 | 0.000e+000 | 0.000e+000 | -81.822 | -82.162 | -0.341 |
| S3O6-2 | 0.000e+000 | 0.000e+000 | -203.395 | -203.736 | -0.341 |
| S4O6-2 | 0.000e+000 | 0.000e+000 | -308.703 | -309.044 | -0.341 |
| S5O6-2 | 0.000e+000 | 0.000e+000 | -443.517 | -443.858 | -0.341 |
| S(5) | 0.000e+000 | | | | |
| S2O5-2 | 0.000e+000 | 0.000e+000 | -113.827 | -114.167 | -0.341 |
| S(6) | 7.308e-003 | | | | |
| SO4-2 | 6.107e-003 | 2.786e-003 | -2.214 | -2.555 | -0.341 |
| CaSO4 | 8.370e-004 | 8.370e-004 | -3.077 | -3.077 | 0.000 |
| NaSO4- | 3.247e-004 | 2.677e-004 | -3.489 | -3.572 | -0.084 |
| KSO4- | 3.939e-005 | 3.247e-005 | -4.405 | -4.488 | -0.084 |
| MgSO4 | 6.254e-009 | 6.254e-009 | -8.204 | -8.204 | 0.000 |
| HSO4- | 8.879e-014 | 7.321e-014 | -13.052 | -13.135 | -0.084 |
| LiSO4- | 1.561e-015 | 1.287e-015 | -14.806 | -14.890 | -0.084 |
| KHSO4 | 6.799e-018 | 6.799e-018 | -17.168 | -17.168 | 0.000 |
| AlSO4+ | 3.289e-029 | 2.712e-029 | -28.483 | -28.567 | -0.084 |
| H2SO4 | 3.153e-029 | 3.153e-029 | -28.501 | -28.501 | 0.000 |
| Al(SO4)2- | 7.113e-030 | 5.865e-030 | -29.148 | -29.232 | -0.084 |
| FeSO4 | 1.823e-033 | 1.823e-033 | -32.739 | -32.739 | 0.000 |
| FeSO4+ | 7.405e-038 | 6.105e-038 | -37.130 | -37.214 | -0.084 |
| Fe(SO4)2- | 5.095e-039 | 4.201e-039 | -38.293 | -38.377 | -0.084 |
| NH4SO4- | 0.000e+000 | 0.000e+000 | -87.439 | -87.523 | -0.084 |
| S(7) | 0.000e+000 | | | | |
| S2O8-2 | 0.000e+000 | 0.000e+000 | -54.738 | -55.079 | -0.341 |
| S(8) | 3.548e-035 | | | | |
| HSO5- | 3.548e-035 | 2.925e-035 | -34.450 | -34.534 | -0.084 |
| Si | 2.272e-005 | | | | |
| HSiO3- | 9.462e-006 | 7.801e-006 | -5.024 | -5.108 | -0.084 |
| H2SiO4-2 | 6.733e-006 | 3.071e-006 | -5.172 | -5.513 | -0.341 |
| NaHSiO3 | 6.497e-006 | 6.497e-006 | -5.187 | -5.187 | 0.000 |
| SiO2 | 3.334e-008 | 3.334e-008 | -7.477 | -7.477 | 0.000 |
| H4(H2SiO4)4-4 | 2.333e-015 | 9.969e-017 | -14.632 | -16.001 | -1.369 |
| H6(H2SiO4)4-2 | 5.179e-019 | 2.363e-019 | -18.286 | -18.627 | -0.341 |

## File 7. Mature Cement, Maximum Ion Content, No Rebar

*INPUT FILE*

```
SOLUTION 1
   temp      15
   pH        7.5 charge
   pe        4
   redox     pe
   units     mmol/kgw
   density   1
   Alkalinity 0
   Cl(-1)    7.5
   Li        1e-010
   Al        1e-010
   Ca        3.1
   Mg        5
   Na        18
   K         1.9
   S(6)      7.3
   N(5)      7.9
   C(4)      21.8
   Br(-1)    0
   Si        0.01
   -water    1 # kg

GAS_PHASE 1
   -fixed_pressure
   -pressure 1
   -volume 1000
   -temperature 25
   CO2(g)    0.056
   O2(g)     0.18
EQUILIBRIUM_PHASES 1
   Brucite   0 1.39
   Ca(OH)2*(CSH(1.5)) 0 9.5
   Calcite   0 0.001
   CSH(1.0-2.5) 0 15.96
   Gibbsite  0 0.001
   goethite  0 1e-005
   SiO2(am)  0 0.02
SAVE solution 1-1
END
```

*SAMPLE OUTPUT, INITIAL CONDITION (FILE 7)*

```
 -------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 1.

-----------------------------Solution composition------------------------------

      Elements           Molality       Moles

      Al              1.000e-013  1.000e-013
      C(4)             2.180e-002  2.180e-002
      Ca               3.100e-003  3.100e-003
      Cl(-1)           7.500e-003  7.500e-003
      K                1.900e-003  1.900e-003
      Li              1.000e-013  1.000e-013
      Mg               5.000e-003  5.000e-003
```

```
N(5)          7.900e-003  7.900e-003
Na            1.800e-002  1.800e-002
S(6)          7.300e-003  7.300e-003
Si            1.000e-005  1.000e-005

----------Description of solution----------

                    pH  =   5.909      Charge balance
                    pe  =   4.000
          Activity of water  =   0.999
             Ionic strength  =  4.415e-002
         Mass of water (kg)  =  1.000e+000
  Total alkalinity (eq/kg)  =  6.100e-003
      Total CO2 (mol/kg)  =  2.180e-002
     Temperature (deg C)  =  15.000
   Electrical balance (eq)  = -1.388e-017
Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
               Iterations  =   8
                  Total H  = 1.110568e+002
                  Total O  = 5.562795e+001
```

*SAMPLE OUTPUT, FINAL TIME STEP (FILE 7)*

```
-------------------------------------------
Beginning of batch-reaction calculations.
-------------------------------------------

Reaction step 1.

Using solution 1.
Using pure phase assemblage 1.
Using gas phase 1.

----------Gas phase----------


Total pressure:   1.0000   atmospheres
   Gas volume:  1.74e+002 liters

                                    Moles in gas
                                -----------------------------------
Component             log P          P     Initial      Final      Delta

CO2(g)              -12.53  2.945e-013  2.289e+000  2.166e-012 -2.289e+000
O2(g)               -0.00  1.000e+000  7.357e+000  7.356e+000 -1.585e-003

----------Phase assemblage----------

                                          Moles in assemblage
Phase               SI log IAP  log KT      Initial       Final       Delta

Brucite           -0.00   16.96   16.96   1.390e+000  1.395e+000  5.000e-003
Ca(OH)2*(CSH(1.5))  -0.00   22.28   22.28   9.500e+000  7.160e+000 -2.340e+000
Calcite            0.00    1.98    1.98   1.000e-003  2.312e+000  2.311e+000
CSH(1.0-2.5)       -0.00   14.80   14.80   1.596e+001  1.598e+001  1.999e-002
Gibbsite           -0.00    8.36    8.36   1.000e-003  3.518e-004 -6.482e-004
Goethite           -0.00    0.91    0.91   1.000e-005  9.995e-006 -5.474e-009
SiO2(am)           -4.60   -7.48   -2.87   2.000e-002           0 -2.000e-002

----------Solution composition----------

      Elements           Molality       Moles
```

| | | |
|---|---|---|
| Al | 6.223e-004 | 6.482e-004 |
| C | 8.212e-006 | 8.553e-006 |
| Ca | 1.170e-002 | 1.219e-002 |
| Cl | 7.200e-003 | 7.500e-003 |
| Fe | 5.256e-009 | 5.474e-009 |
| K | 1.824e-003 | 1.900e-003 |
| Li | 9.600e-014 | 1.000e-013 |
| Mg | 4.942e-008 | 5.147e-008 |
| N | 7.584e-003 | 7.900e-003 |
| Na | 1.728e-002 | 1.800e-002 |
| S | 7.008e-003 | 7.300e-003 |
| Si | 1.528e-005 | 1.591e-005 |

----------Description of solution----------

pH = 12.328 Charge balance
pe = 9.199 Adjusted to redox equilibrium
Activity of water = 0.999
Ionic strength = 5.181e-002
Mass of water (kg) = 1.042e+000
Total alkalinity (eq/kg) = 1.557e-002
Total CO2 (mol/kg) = 8.212e-006
Temperature (deg C) = 15.000
Electrical balance (eq) = 1.017e-015
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 0.00
Iterations = 63
Total H = 1.156882e+002
Total O = 5.790833e+001

----------Distribution of species----------

| Species | Molality | Log Activity | Log Molality | Log Activity | Gamma |
|---|---|---|---|---|---|
| OH- | 1.148e-002 | 9.350e-003 | -1.940 | -2.029 | -0.089 |
| H+ | 5.481e-013 | 4.701e-013 | -12.261 | -12.328 | -0.067 |
| H2O | 5.553e+001 | 9.989e-001 | 1.744 | -0.000 | 0.000 |
| Al | 6.223e-004 | | | | |
| AlO2- | 6.211e-004 | 5.090e-004 | -3.207 | -3.293 | -0.086 |
| NaAlO2 | 1.180e-006 | 1.180e-006 | -5.928 | -5.928 | 0.000 |
| HAlO2 | 1.166e-009 | 1.166e-009 | -8.933 | -8.933 | 0.000 |
| Al(OH)2+ | 8.780e-016 | 7.196e-016 | -15.057 | -15.143 | -0.086 |
| AlOH+2 | 6.330e-022 | 2.881e-022 | -21.199 | -21.540 | -0.342 |
| Al+3 | 9.982e-029 | 2.414e-029 | -28.001 | -28.617 | -0.616 |
| AlSO4+ | 7.204e-029 | 5.904e-029 | -28.142 | -28.229 | -0.086 |
| Al(SO4)2- | 1.336e-029 | 1.095e-029 | -28.874 | -28.960 | -0.086 |
| Al2(OH)2+4 | 1.074e-039 | 0.000e+000 | -38.969 | -40.270 | -1.301 |
| Al3(OH)4+5 | 0.000e+000 | 0.000e+000 | -48.441 | -50.423 | -1.981 |
| Al13O4(OH)24+7 | 0.000e+000 | 0.000e+000 | -72.392 | -76.277 | -3.885 |
| C(-2) | 0.000e+000 | | | | |
| C2H4 | 0.000e+000 | 0.000e+000 | -295.796 | -295.796 | 0.000 |
| C(-3) | 0.000e+000 | | | | |
| C2H6 | 0.000e+000 | 0.000e+000 | -267.647 | -267.647 | 0.000 |
| C(-4) | 0.000e+000 | | | | |
| CH4 | 0.000e+000 | 0.000e+000 | -164.002 | -164.002 | 0.000 |
| C(2) | 0.000e+000 | | | | |
| CO | 0.000e+000 | 0.000e+000 | -62.235 | -62.235 | 0.000 |
| C(4) | 8.212e-006 | | | | |
| CaCO3 | 6.322e-006 | 6.322e-006 | -5.199 | -5.199 | 0.000 |
| CO3-2 | 1.812e-006 | 8.247e-007 | -5.742 | -6.084 | -0.342 |
| NaCO3- | 6.337e-008 | 5.194e-008 | -7.198 | -7.285 | -0.086 |

| | | | | | |
|---|---|---|---|---|---|
| HCO3- | 1.315e-008 | 1.078e-008 | -7.881 | -7.967 | -0.086 |
| CaHCO3+ | 6.439e-010 | 5.277e-010 | -9.191 | -9.278 | -0.086 |
| NaHCO3 | 2.596e-010 | 2.596e-010 | -9.586 | -9.586 | 0.000 |
| MgCO3 | 1.540e-011 | 1.540e-011 | -10.813 | -10.813 | 0.000 |
| CO2 | 1.348e-014 | 1.365e-014 | -13.870 | -13.865 | 0.005 |
| MgHCO3+ | 3.041e-015 | 2.492e-015 | -14.517 | -14.603 | -0.086 |
| FeCO3+ | 1.223e-032 | 1.003e-032 | -31.912 | -31.999 | -0.086 |
| FeCO3 | 4.436e-034 | 4.436e-034 | -33.353 | -33.353 | 0.000 |
| FeHCO3+ | 5.301e-038 | 4.345e-038 | -37.276 | -37.362 | -0.086 |
| Ca | 1.170e-002 | | | | |
| Ca+2 | 8.662e-003 | 4.191e-003 | -2.062 | -2.378 | -0.315 |
| CaOH+ | 1.535e-003 | 1.258e-003 | -2.814 | -2.900 | -0.086 |
| CaSO4 | 1.336e-003 | 1.336e-003 | -2.874 | -2.874 | 0.000 |
| CaNO3+ | 1.541e-004 | 1.263e-004 | -3.812 | -3.898 | -0.086 |
| CaCO3 | 6.322e-006 | 6.322e-006 | -5.199 | -5.199 | 0.000 |
| CaCl+ | 6.140e-006 | 5.032e-006 | -5.212 | -5.298 | -0.086 |
| CaCl2 | 3.835e-008 | 3.835e-008 | -7.416 | -7.416 | 0.000 |
| CaHCO3+ | 6.439e-010 | 5.277e-010 | -9.191 | -9.278 | -0.086 |
| Cl(-1) | 7.200e-003 | | | | |
| Cl- | 7.181e-003 | 5.813e-003 | -2.144 | -2.236 | -0.092 |
| NaCl | 1.317e-005 | 1.317e-005 | -4.880 | -4.880 | 0.000 |
| CaCl+ | 6.140e-006 | 5.032e-006 | -5.212 | -5.298 | -0.086 |
| KCl | 2.286e-007 | 2.286e-007 | -6.641 | -6.641 | 0.000 |
| CaCl2 | 3.835e-008 | 3.835e-008 | -7.416 | -7.416 | 0.000 |
| MgCl+ | 1.144e-010 | 9.380e-011 | -9.941 | -10.028 | -0.086 |
| HCl | 6.022e-016 | 6.022e-016 | -15.220 | -15.220 | 0.000 |
| LiCl | 1.352e-017 | 1.352e-017 | -16.869 | -16.869 | 0.000 |
| FeCl+ | 3.813e-035 | 3.126e-035 | -34.419 | -34.505 | -0.086 |
| FeCl2+ | 4.670e-039 | 3.828e-039 | -38.331 | -38.417 | -0.086 |
| FeCl+2 | 1.069e-039 | 4.868e-040 | -38.971 | -39.313 | -0.342 |
| FeCl2 | 9.267e-040 | 9.267e-040 | -39.033 | -39.033 | 0.000 |
| FeCl4-2 | 0.000e+000 | 0.000e+000 | -42.698 | -43.049 | -0.352 |
| FeCl4- | 0.000e+000 | 0.000e+000 | -45.722 | -45.808 | -0.086 |
| Cl(1) | 8.526e-020 | | | | |
| ClO- | 8.526e-020 | 6.988e-020 | -19.069 | -19.156 | -0.086 |
| HClO | 1.218e-024 | 1.218e-024 | -23.914 | -23.914 | 0.000 |
| Cl(3) | 1.700e-029 | | | | |
| ClO2- | 1.700e-029 | 1.394e-029 | -28.769 | -28.856 | -0.086 |
| HClO2 | 9.685e-039 | 9.685e-039 | -38.014 | -38.014 | 0.000 |
| Cl(5) | 7.302e-025 | | | | |
| ClO3- | 7.302e-025 | 5.949e-025 | -24.137 | -24.226 | -0.089 |
| Cl(7) | 1.307e-024 | | | | |
| ClO4- | 1.307e-024 | 1.065e-024 | -23.884 | -23.973 | -0.089 |
| Fe(2) | 9.119e-027 | | | | |
| Fe(OH)3- | 8.991e-027 | 7.369e-027 | -26.046 | -26.133 | -0.086 |
| Fe(OH)2 | 8.711e-029 | 8.711e-029 | -28.060 | -28.060 | 0.000 |
| Fe(OH)4-2 | 3.519e-029 | 1.566e-029 | -28.454 | -28.805 | -0.352 |
| FeOH+ | 6.297e-030 | 5.161e-030 | -29.201 | -29.287 | -0.086 |
| Fe+2 | 1.587e-032 | 7.680e-033 | -31.799 | -32.115 | -0.315 |
| FeSO4 | 2.909e-033 | 2.909e-033 | -32.536 | -32.536 | 0.000 |
| FeCO3 | 4.436e-034 | 4.436e-034 | -33.353 | -33.353 | 0.000 |
| FeCl+ | 3.813e-035 | 3.126e-035 | -34.419 | -34.505 | -0.086 |
| FeHCO3+ | 5.301e-038 | 4.345e-038 | -37.276 | -37.362 | -0.086 |
| FeCl2 | 9.267e-040 | 9.267e-040 | -39.033 | -39.033 | 0.000 |
| FeCl4-2 | 0.000e+000 | 0.000e+000 | -42.698 | -43.049 | -0.352 |
| Fe(3) | 5.256e-009 | | | | |
| Fe(OH)4- | 5.248e-009 | 4.301e-009 | -8.280 | -8.366 | -0.086 |
| Fe(OH)3 | 8.058e-012 | 8.058e-012 | -11.094 | -11.094 | 0.000 |
| Fe(OH)2+ | 9.892e-018 | 8.107e-018 | -17.005 | -17.091 | -0.086 |
| FeOH+2 | 2.532e-026 | 1.152e-026 | -25.597 | -25.938 | -0.342 |
| FeCO3+ | 1.223e-032 | 1.003e-032 | -31.912 | -31.999 | -0.086 |
| Fe+3 | 3.472e-036 | 8.398e-037 | -35.459 | -36.076 | -0.616 |

| | | | | | |
|---|---|---|---|---|---|
| FeSO4+ | 1.622e-037 | 1.329e-037 | -36.790 | -36.876 | -0.086 |
| FeNO3+2 | 1.110e-037 | 5.051e-038 | -36.955 | -37.297 | -0.342 |
| Fe(SO4)2- | 9.573e-039 | 7.846e-039 | -38.019 | -38.105 | -0.086 |
| FeCl2+ | 4.670e-039 | 3.828e-039 | -38.331 | -38.417 | -0.086 |
| FeCl+2 | 1.069e-039 | 4.868e-040 | -38.971 | -39.313 | -0.342 |
| FeCl4- | 0.000e+000 | 0.000e+000 | -45.722 | -45.808 | -0.086 |
| Fe2(OH)2+4 | 0.000e+000 | 0.000e+000 | -49.146 | -50.447 | -1.301 |
| FeNO2+2 | 0.000e+000 | 0.000e+000 | -49.213 | -49.555 | -0.342 |
| Fe3(OH)4+5 | 0.000e+000 | 0.000e+000 | -63.237 | -65.218 | -1.981 |
| H(0) | 0.000e+000 | | | | |
| H2 | 0.000e+000 | 0.000e+000 | -46.369 | -46.363 | 0.005 |
| K | 1.824e-003 | | | | |
| K+ | 1.781e-003 | 1.441e-003 | -2.749 | -2.841 | -0.092 |
| KSO4- | 3.254e-005 | 2.667e-005 | -4.488 | -4.574 | -0.086 |
| KOH | 1.062e-005 | 1.062e-005 | -4.974 | -4.974 | 0.000 |
| KCl | 2.286e-007 | 2.286e-007 | -6.641 | -6.641 | 0.000 |
| KHSO4 | 7.617e-018 | 7.617e-018 | -17.118 | -17.118 | 0.000 |
| Li | 9.600e-014 | | | | |
| Li+ | 9.098e-014 | 7.614e-014 | -13.041 | -13.118 | -0.077 |
| LiOH | 3.707e-015 | 3.707e-015 | -14.431 | -14.431 | 0.000 |
| LiSO4- | 1.307e-015 | 1.072e-015 | -14.884 | -14.970 | -0.086 |
| LiCl | 1.352e-017 | 1.352e-017 | -16.869 | -16.869 | 0.000 |
| Mg | 4.942e-008 | | | | |
| Mg+2 | 3.930e-008 | 2.036e-008 | -7.406 | -7.691 | -0.286 |
| MgSO4 | 9.982e-009 | 9.982e-009 | -8.001 | -8.001 | 0.000 |
| MgCl+ | 1.144e-010 | 9.380e-011 | -9.941 | -10.028 | -0.086 |
| MgCO3 | 1.540e-011 | 1.540e-011 | -10.813 | -10.813 | 0.000 |
| MgHCO3+ | 3.041e-015 | 2.492e-015 | -14.517 | -14.603 | -0.086 |
| Mg4(OH)4+4 | 1.245e-020 | 6.230e-022 | -19.905 | -21.206 | -1.301 |
| N(-03) | 0.000e+000 | | | | |
| N3- | 0.000e+000 | 0.000e+000 | -112.637 | -112.724 | -0.086 |
| HN3 | 0.000e+000 | 0.000e+000 | -120.257 | -120.257 | 0.000 |
| N(-3) | 0.000e+000 | | | | |
| NH3 | 0.000e+000 | 0.000e+000 | -73.335 | -73.335 | 0.000 |
| NH4+ | 0.000e+000 | 0.000e+000 | -76.014 | -76.108 | -0.095 |
| NH4SO4- | 0.000e+000 | 0.000e+000 | -87.258 | -87.345 | -0.086 |
| N(0) | 1.111e-030 | | | | |
| N2 | 5.555e-031 | 5.555e-031 | -30.255 | -30.255 | 0.000 |
| N(3) | 2.904e-017 | | | | |
| NO2- | 2.904e-017 | 2.351e-017 | -16.537 | -16.629 | -0.092 |
| HNO2 | 2.337e-026 | 2.337e-026 | -25.631 | -25.631 | 0.000 |
| FeNO2+2 | 0.000e+000 | 0.000e+000 | -49.213 | -49.555 | -0.342 |
| N(5) | 7.584e-003 | | | | |
| NO3- | 7.430e-003 | 6.015e-003 | -2.129 | -2.221 | -0.092 |
| CaNO3+ | 1.541e-004 | 1.263e-004 | -3.812 | -3.898 | -0.086 |
| HNO3 | 1.163e-016 | 1.163e-016 | -15.934 | -15.934 | 0.000 |
| FeNO3+2 | 1.110e-037 | 5.051e-038 | -36.955 | -37.297 | -0.342 |
| Na | 1.728e-002 | | | | |
| Na+ | 1.697e-002 | 1.391e-002 | -1.770 | -1.857 | -0.086 |
| NaSO4- | 2.680e-004 | 2.196e-004 | -3.572 | -3.658 | -0.086 |
| NaOH | 2.299e-005 | 2.299e-005 | -4.638 | -4.638 | 0.000 |
| NaCl | 1.317e-005 | 1.317e-005 | -4.880 | -4.880 | 0.000 |
| NaHSiO3 | 4.555e-006 | 4.555e-006 | -5.342 | -5.342 | 0.000 |
| NaAlO2 | 1.180e-006 | 1.180e-006 | -5.928 | -5.928 | 0.000 |
| NaCO3- | 6.337e-008 | 5.194e-008 | -7.198 | -7.285 | -0.086 |
| NaHCO3 | 2.596e-010 | 2.596e-010 | -9.586 | -9.586 | 0.000 |
| O(0) | 3.043e-003 | | | | |
| O2 | 1.521e-003 | 1.541e-003 | -2.818 | -2.812 | 0.005 |
| S(-2) | 0.000e+000 | | | | |
| HS- | 0.000e+000 | 0.000e+000 | -152.786 | -152.875 | -0.089 |
| S-2 | 0.000e+000 | 0.000e+000 | -153.441 | -153.774 | -0.333 |
| H2S | 0.000e+000 | 0.000e+000 | -158.052 | -158.052 | 0.000 |

```
  S2-2              0.000e+000  0.000e+000  -272.226  -272.578    -0.352
  S3-2              0.000e+000  0.000e+000  -391.068  -391.420    -0.352
  S4-2              0.000e+000  0.000e+000  -510.140  -510.492    -0.352
  S5-2              0.000e+000  0.000e+000  -629.439  -629.791    -0.352
S(2)         0.000e+000
  S2O3-2            0.000e+000  0.000e+000  -162.594  -162.945    -0.352
  HS2O3-            0.000e+000  0.000e+000  -174.173  -174.259    -0.086
S(3)         0.000e+000
  S2O4-2            0.000e+000  0.000e+000  -148.260  -148.593    -0.333
S(4)         0.000e+000
  SO3-2             0.000e+000  0.000e+000   -49.120   -49.461    -0.342
  HSO3-             0.000e+000  0.000e+000   -54.525   -54.611    -0.086
  H2SO3             0.000e+000  0.000e+000   -64.904   -64.904     0.000
  SO2               0.000e+000  0.000e+000   -65.157   -65.157     0.000
  S2O6-2            0.000e+000  0.000e+000   -81.674   -82.026    -0.352
  S3O6-2            0.000e+000  0.000e+000  -203.045  -203.396    -0.352
  S4O6-2            0.000e+000  0.000e+000  -308.150  -308.502    -0.352
  S5O6-2            0.000e+000  0.000e+000  -442.760  -443.112    -0.352
S(5)         0.000e+000
  S2O5-2            0.000e+000  0.000e+000  -113.679  -114.031    -0.352
S(6)         7.008e-003
  SO4-2             5.372e-003  2.390e-003    -2.270    -2.622    -0.352
  CaSO4             1.336e-003  1.336e-003    -2.874    -2.874     0.000
  NaSO4-            2.680e-004  2.196e-004    -3.572    -3.658    -0.086
  KSO4-             3.254e-005  2.667e-005    -4.488    -4.574    -0.086
  MgSO4             9.982e-009  9.982e-009    -8.001    -8.001     0.000
  HSO4-             1.045e-013  8.567e-014   -12.981   -13.067    -0.086
  LiSO4-            1.307e-015  1.072e-015   -14.884   -14.970    -0.086
  KHSO4             7.617e-018  7.617e-018   -17.118   -17.118     0.000
  AlSO4+            7.204e-029  5.904e-029   -28.142   -28.229    -0.086
  H2SO4             5.033e-029  5.033e-029   -28.298   -28.298     0.000
  Al(SO4)2-         1.336e-029  1.095e-029   -28.874   -28.960    -0.086
  FeSO4             2.909e-033  2.909e-033   -32.536   -32.536     0.000
  FeSO4+            1.622e-037  1.329e-037   -36.790   -36.876    -0.086
  Fe(SO4)2-         9.573e-039  7.846e-039   -38.019   -38.105    -0.086
  NH4SO4-           0.000e+000  0.000e+000   -87.258   -87.345    -0.086
S(7)         0.000e+000
  S2O8-2            0.000e+000  0.000e+000   -54.591   -54.942    -0.352
S(8)         4.177e-035
  HSO5-             4.177e-035  3.423e-035   -34.379   -34.466    -0.086
Si           1.528e-005
  HSiO3-            6.978e-006  5.720e-006    -5.156    -5.243    -0.086
  NaHSiO3           4.555e-006  4.555e-006    -5.342    -5.342     0.000
  H2SiO4-2          3.710e-006  1.651e-006    -5.431    -5.782    -0.352
  SiO2              3.334e-008  3.334e-008    -7.477    -7.477     0.000
  H4(H2SiO4)4-4     7.456e-016  2.880e-017   -15.127   -16.541    -1.413
  H6(H2SiO4)4-2     2.855e-019  1.270e-019   -18.544   -18.896    -0.352
```

## File 8. Mature Cement, Maximum Ion Content, With Rebar

*INPUT FILE*

```
SOLUTION 1
    temp      15
    pH        7.5
    pe        4
    redox     pe
    units     mmol/kgw
    density   1
    Alkalinity 0
    Cl(-1)    7.5
    Li        1e-010
```

```
    Al       1e-010
    Ca       3.1
    Mg       5
    Na       18
    K        1.9
    S(6)     7.3
    N(5)     7.9
    C(4)     21.8
    Br(-1)   0
    Si       0.01
    -water   1 # kg

GAS_PHASE 1
    -fixed_pressure
    -pressure 1
    -volume 1000
    -temperature 25
    CO2(g)   0.056
    O2(g)    0.18
EQUILIBRIUM_PHASES 1
    Brucite   0 1.39
    Ca(OH)2*(CSH(1.5)) 0 9.5
    Calcite   0 0.001
    CSH(1.0-2.5) 0 15.96
    Gibbsite  0 0.001
    goethite  0 1e-005
    SiO2(am)  0 0.02
REACTION 1
    Fe       1
    4.75 moles in 60 steps
SAVE solution 1-1
END
```

## *SAMPLE OUTPUT, INITIAL CONDITION (FILE 8)*

```
-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 1.

-----------------------------Solution composition------------------------------

      Elements          Molality       Moles

      Al              1.000e-013  1.000e-013
      C(4)             2.180e-002  2.180e-002
      Ca               3.100e-003  3.100e-003
      Cl(-1)           7.500e-003  7.500e-003
      K               1.900e-003  1.900e-003
      Li              1.000e-013  1.000e-013
      Mg               5.000e-003  5.000e-003
      N(5)             7.900e-003  7.900e-003
      Na               1.800e-002  1.800e-002
      S(6)             7.300e-003  7.300e-003
      Si              1.000e-005  1.000e-005

----------------------------Description of solution----------------------------

                                pH  =   7.500
                                pe  =   4.000
                    Activity of water  =   0.999
```

Ionic strength = 5.066e-002
Mass of water (kg) = 1.000e+000
Total alkalinity (eq/kg) = 2.058e-002
Total CO2 (mol/kg) = 2.180e-002
Temperature (deg C) = 15.000
Electrical balance (eq) = -1.448e-002
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -18.54
Iterations = 4
Total H = 1.110710e+002
Total O = 5.564231e+001

## *SAMPLE OUTPUT, FINAL TIME STEP (FILE 8)*

Reaction step 60.

Using solution 1.
Using pure phase assemblage 1.
Using gas phase 1.
Using reaction 1.

Reaction 1. Irreversible reaction defined in simulation 1.

4.750e+000 moles of the following reaction have been added:

| Reactant | Relative moles |
|---|---|
| Fe | 1.00000 |

| Element | Relative moles |
|---|---|
| Fe | 1.00000 |

----------Gas phase----------

Total pressure: 1.0000 atmospheres
Gas volume: 8.97e+001 liters

| Component | log P | P | Moles in gas: Initial | Final | Delta |
|---|---|---|---|---|---|
| CO2(g) | -12.53 | 2.945e-013 | 2.289e+000 | 1.117e-012 | -2.289e+000 |
| O2(g) | 0.00 | 1.000e+000 | 7.357e+000 | 3.793e+000 | -3.564e+000 |

----------Phase assemblage----------

| Phase | SI | log IAP | log KT | Moles in assemblage: Initial | Final | Delta |
|---|---|---|---|---|---|---|
| Brucite | 0.00 | 16.96 | 16.96 | 1.390e+000 | 1.395e+000 | 5.000e-003 |
| Ca(OH)2*(CSH(1.5)) | 0.00 | 22.28 | 22.28 | 9.500e+000 | 7.166e+000 | -2.334e+000 |
| Calcite | 0.00 | 1.98 | 1.98 | 1.000e-003 | 2.312e+000 | 2.311e+000 |
| CSH(1.0-2.5) | 0.00 | 14.80 | 14.80 | 1.596e+001 | 1.598e+001 | 1.999e-002 |
| Gibbsite | 0.00 | 8.36 | 8.36 | 1.000e-003 | 1.571e-004 | -8.429e-004 |
| Goethite | -0.00 | 0.91 | 0.91 | 1.000e-005 | 4.750e+000 | 4.750e+000 |
| SiO2(am) | -4.60 | -7.48 | -2.87 | 2.000e-002 | 0 | -2.000e-002 |

----------Solution composition----------

| Elements | Molality | Moles |
|---|---|---|

| | | |
|---|---|---|
| Al | 8.438e-004 | 8.429e-004 |
| C | 9.756e-006 | 9.745e-006 |
| Ca | 6.616e-003 | 6.608e-003 |
| Cl | 7.508e-003 | 7.500e-003 |
| Fe | 7.123e-009 | 7.115e-009 |
| K | 1.902e-003 | 1.900e-003 |
| Li | 1.001e-013 | 1.000e-013 |
| Mg | 2.711e-008 | 2.708e-008 |
| N | 7.909e-003 | 7.900e-003 |
| Na | 1.802e-002 | 1.800e-002 |
| S | 7.308e-003 | 7.300e-003 |
| Si | 2.272e-005 | 2.270e-005 |

----------Description of solution----------

pH = 12.463 Charge balance
pe = 9.065 Adjusted to redox equilibrium
Activity of water = 0.999
Ionic strength = 4.775e-002
Mass of water (kg) = 9.989e-001
Total alkalinity (eq/kg) = 2.015e-002
Total CO2 (mol/kg) = 9.756e-006
Temperature (deg C) = 15.000
Electrical balance (eq) = -1.448e-002
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -19.55
Iterations = 74
Total H = 1.109419e+002
Total O = 5.553702e+001

----------Distribution of species----------

| Species | Molality | Log Activity | Log Molality | Log Activity | Gamma |
|---|---|---|---|---|---|
| OH- | 1.555e-002 | 1.275e-002 | -1.808 | -1.894 | -0.086 |
| H+ | 4.004e-013 | 3.446e-013 | -12.397 | -12.463 | -0.065 |
| H2O | 5.553e+001 | 9.989e-001 | 1.744 | -0.000 | 0.000 |
| Al | 8.438e-004 | | | | |
| AlO2- | 8.421e-004 | 6.944e-004 | -3.075 | -3.158 | -0.084 |
| NaAlO2 | 1.683e-006 | 1.683e-006 | -5.774 | -5.774 | 0.000 |
| HAlO2 | 1.166e-009 | 1.166e-009 | -8.933 | -8.933 | 0.000 |
| Al(OH)2+ | 6.399e-016 | 5.276e-016 | -15.194 | -15.278 | -0.084 |
| AlOH+2 | 3.323e-022 | 1.548e-022 | -21.478 | -21.810 | -0.332 |
| Al+3 | 3.801e-029 | 9.514e-030 | -28.420 | -29.022 | -0.602 |
| AlSO4+ | 3.289e-029 | 2.712e-029 | -28.483 | -28.567 | -0.084 |
| Al(SO4)2- | 7.113e-030 | 5.865e-030 | -29.148 | -29.232 | -0.084 |
| Al2(OH)2+4 | 2.848e-040 | 0.000e+000 | -39.546 | -40.809 | -1.264 |
| Al3(OH)4+5 | 0.000e+000 | 0.000e+000 | -49.171 | -51.097 | -1.926 |
| Al13O4(OH)24+7 | 0.000e+000 | 0.000e+000 | -73.444 | -77.221 | -3.777 |
| C(-2) | 0.000e+000 | | | | |
| C2H4 | 0.000e+000 | 0.000e+000 | -295.796 | -295.796 | 0.000 |
| C(-3) | 0.000e+000 | | | | |
| C2H6 | 0.000e+000 | 0.000e+000 | -267.647 | -267.647 | 0.000 |
| C(-4) | 0.000e+000 | | | | |
| CH4 | 0.000e+000 | 0.000e+000 | -164.002 | -164.002 | 0.000 |
| C(2) | 0.000e+000 | | | | |
| CO | 0.000e+000 | 0.000e+000 | -62.235 | -62.235 | 0.000 |
| C(4) | 9.756e-006 | | | | |
| CaCO3 | 6.322e-006 | 6.322e-006 | -5.199 | -5.199 | 0.000 |
| CO3-2 | 3.293e-006 | 1.534e-006 | -5.482 | -5.814 | -0.332 |
| NaCO3- | 1.225e-007 | 1.010e-007 | -6.912 | -6.996 | -0.084 |

| | | | | | |
|---|---|---|---|---|---|
| HCO3- | 1.783e-008 | 1.470e-008 | -7.749 | -7.833 | -0.084 |
| CaHCO3+ | 4.693e-010 | 3.869e-010 | -9.329 | -9.412 | -0.084 |
| NaHCO3 | 3.703e-010 | 3.703e-010 | -9.431 | -9.431 | 0.000 |
| MgCO3 | 1.540e-011 | 1.540e-011 | -10.813 | -10.813 | 0.000 |
| CO2 | 1.349e-014 | 1.365e-014 | -13.870 | -13.865 | 0.005 |
| MgHCO3+ | 2.216e-015 | 1.827e-015 | -14.654 | -14.738 | -0.084 |
| FeCO3+ | 8.915e-033 | 7.350e-033 | -32.050 | -32.134 | -0.084 |
| FeCO3 | 4.436e-034 | 4.436e-034 | -33.353 | -33.353 | 0.000 |
| FeHCO3+ | 3.863e-038 | 3.185e-038 | -37.413 | -37.497 | -0.084 |
| Ca | 6.616e-003 | | | | |
| Ca+2 | 4.563e-003 | 2.253e-003 | -2.341 | -2.647 | -0.307 |
| CaOH+ | 1.119e-003 | 9.223e-004 | -2.951 | -3.035 | -0.084 |
| CaSO4 | 8.370e-004 | 8.370e-004 | -3.077 | -3.077 | 0.000 |
| CaNO3+ | 8.729e-005 | 7.197e-005 | -4.059 | -4.143 | -0.084 |
| CaCO3 | 6.322e-006 | 6.322e-006 | -5.199 | -5.199 | 0.000 |
| CaCl+ | 3.445e-006 | 2.841e-006 | -5.463 | -5.547 | -0.084 |
| CaCl2 | 2.273e-008 | 2.273e-008 | -7.643 | -7.643 | 0.000 |
| CaHCO3+ | 4.693e-010 | 3.869e-010 | -9.329 | -9.412 | -0.084 |
| Cl(-1) | 7.508e-003 | | | | |
| Cl- | 7.490e-003 | 6.104e-003 | -2.126 | -2.214 | -0.089 |
| NaCl | 1.446e-005 | 1.446e-005 | -4.840 | -4.840 | 0.000 |
| CaCl+ | 3.445e-006 | 2.841e-006 | -5.463 | -5.547 | -0.084 |
| KCl | 2.508e-007 | 2.508e-007 | -6.601 | -6.601 | 0.000 |
| CaCl2 | 2.273e-008 | 2.273e-008 | -7.643 | -7.643 | 0.000 |
| MgCl+ | 6.422e-011 | 5.295e-011 | -10.192 | -10.276 | -0.084 |
| HCl | 4.637e-016 | 4.637e-016 | -15.334 | -15.334 | 0.000 |
| LiCl | 1.464e-017 | 1.464e-017 | -16.835 | -16.835 | 0.000 |
| FeCl+ | 2.140e-035 | 1.764e-035 | -34.670 | -34.753 | -0.084 |
| FeCl2+ | 2.018e-039 | 1.664e-039 | -38.695 | -38.779 | -0.084 |
| FeCl2 | 5.493e-040 | 5.493e-040 | -39.260 | -39.260 | 0.000 |
| FeCl+2 | 4.323e-040 | 2.014e-040 | -39.364 | -39.696 | -0.332 |
| FeCl4-2 | 0.000e+000 | 0.000e+000 | -42.893 | -43.234 | -0.341 |
| FeCl4- | 0.000e+000 | 0.000e+000 | -46.044 | -46.128 | -0.084 |
| Cl(1) | 8.901e-020 | | | | |
| ClO- | 8.901e-020 | 7.339e-020 | -19.051 | -19.134 | -0.084 |
| HClO | 9.379e-025 | 9.379e-025 | -24.028 | -24.028 | 0.000 |
| Cl(3) | 1.775e-029 | | | | |
| ClO2- | 1.775e-029 | 1.463e-029 | -28.751 | -28.835 | -0.084 |
| HClO2 | 7.457e-039 | 7.457e-039 | -38.127 | -38.127 | 0.000 |
| Cl(5) | 7.620e-025 | | | | |
| ClO3- | 7.620e-025 | 6.248e-025 | -24.118 | -24.204 | -0.086 |
| Cl(7) | 1.364e-024 | | | | |
| ClO4- | 1.364e-024 | 1.119e-024 | -23.865 | -23.951 | -0.086 |
| Fe(2) | 1.235e-026 | | | | |
| Fe(OH)3- | 1.219e-026 | 1.005e-026 | -25.914 | -25.998 | -0.084 |
| Fe(OH)2 | 8.711e-029 | 8.711e-029 | -28.060 | -28.060 | 0.000 |
| Fe(OH)4-2 | 6.386e-029 | 2.913e-029 | -28.195 | -28.536 | -0.341 |
| FeOH+ | 4.589e-030 | 3.784e-030 | -29.338 | -29.422 | -0.084 |
| Fe+2 | 8.362e-033 | 4.128e-033 | -32.078 | -32.384 | -0.307 |
| FeSO4 | 1.823e-033 | 1.823e-033 | -32.739 | -32.739 | 0.000 |
| FeCO3 | 4.436e-034 | 4.436e-034 | -33.353 | -33.353 | 0.000 |
| FeCl+ | 2.140e-035 | 1.764e-035 | -34.670 | -34.753 | -0.084 |
| FeHCO3+ | 3.863e-038 | 3.185e-038 | -37.413 | -37.497 | -0.084 |
| FeCl2 | 5.493e-040 | 5.493e-040 | -39.260 | -39.260 | 0.000 |
| FeCl4-2 | 0.000e+000 | 0.000e+000 | -42.893 | -43.234 | -0.341 |
| Fe(3) | 7.123e-009 | | | | |
| Fe(OH)4- | 7.115e-009 | 5.866e-009 | -8.148 | -8.232 | -0.084 |
| Fe(OH)3 | 8.058e-012 | 8.058e-012 | -11.094 | -11.094 | 0.000 |
| Fe(OH)2+ | 7.209e-018 | 5.944e-018 | -17.142 | -17.226 | -0.084 |
| FeOH+2 | 1.329e-026 | 6.193e-027 | -25.876 | -26.208 | -0.332 |
| FeCO3+ | 8.915e-033 | 7.350e-033 | -32.050 | -32.134 | -0.084 |
| Fe+3 | 1.322e-036 | 3.310e-037 | -35.879 | -36.480 | -0.602 |

| | | | | | |
|---|---|---|---|---|---|
| FeSO4+ | 7.405e-038 | 6.105e-038 | -37.130 | -37.214 | -0.084 |
| FeNO3+2 | 4.527e-038 | 2.110e-038 | -37.344 | -37.676 | -0.332 |
| Fe(SO4)2- | 5.095e-039 | 4.201e-039 | -38.293 | -38.377 | -0.084 |
| FeCl2+ | 2.018e-039 | 1.664e-039 | -38.695 | -38.779 | -0.084 |
| FeCl+2 | 4.323e-040 | 2.014e-040 | -39.364 | -39.696 | -0.332 |
| FeCl4- | 0.000e+000 | 0.000e+000 | -46.044 | -46.128 | -0.084 |
| FeNO2+2 | 0.000e+000 | 0.000e+000 | -49.602 | -49.934 | -0.332 |
| Fe2(OH)2+4 | 0.000e+000 | 0.000e+000 | -49.723 | -50.986 | -1.264 |
| Fe3(OH)4+5 | 0.000e+000 | 0.000e+000 | -63.966 | -65.892 | -1.926 |
| H(0) | 0.000e+000 | | | | |
| H2 | 0.000e+000 | 0.000e+000 | -46.369 | -46.364 | 0.005 |
| K | 1.902e-003 | | | | |
| K+ | 1.847e-003 | 1.506e-003 | -2.733 | -2.822 | -0.089 |
| KSO4- | 3.939e-005 | 3.247e-005 | -4.405 | -4.488 | -0.084 |
| KOH | 1.513e-005 | 1.513e-005 | -4.820 | -4.820 | 0.000 |
| KCl | 2.508e-007 | 2.508e-007 | -6.601 | -6.601 | 0.000 |
| KHSO4 | 6.799e-018 | 6.799e-018 | -17.168 | -17.168 | 0.000 |
| Li | 1.001e-013 | | | | |
| Li+ | 9.333e-014 | 7.848e-014 | -13.030 | -13.105 | -0.075 |
| LiOH | 5.211e-015 | 5.211e-015 | -14.283 | -14.283 | 0.000 |
| LiSO4- | 1.561e-015 | 1.287e-015 | -14.806 | -14.890 | -0.084 |
| LiCl | 1.464e-017 | 1.464e-017 | -16.835 | -16.835 | 0.000 |
| Mg | 2.711e-008 | | | | |
| Mg+2 | 2.078e-008 | 1.094e-008 | -7.682 | -7.961 | -0.279 |
| MgSO4 | 6.254e-009 | 6.254e-009 | -8.204 | -8.204 | 0.000 |
| MgCl+ | 6.422e-011 | 5.295e-011 | -10.192 | -10.276 | -0.084 |
| MgCO3 | 1.540e-011 | 1.540e-011 | -10.813 | -10.813 | 0.000 |
| MgHCO3+ | 2.216e-015 | 1.827e-015 | -14.654 | -14.738 | -0.084 |
| Mg4(OH)4+4 | 3.303e-021 | 1.800e-022 | -20.481 | -21.745 | -1.264 |
| N(-03) | 0.000e+000 | | | | |
| N3- | 0.000e+000 | 0.000e+000 | -112.834 | -112.918 | -0.084 |
| HN3 | 0.000e+000 | 0.000e+000 | -120.585 | -120.585 | 0.000 |
| N(-3) | 0.000e+000 | | | | |
| NH3 | 0.000e+000 | 0.000e+000 | -73.445 | -73.445 | 0.000 |
| NH4+ | 0.000e+000 | 0.000e+000 | -76.261 | -76.353 | -0.092 |
| NH4SO4- | 0.000e+000 | 0.000e+000 | -87.439 | -87.523 | -0.084 |
| N(0) | 6.707e-031 | | | | |
| N2 | 3.353e-031 | 3.353e-031 | -30.475 | -30.475 | 0.000 |
| N(3) | 3.057e-017 | | | | |
| NO2- | 3.057e-017 | 2.491e-017 | -16.515 | -16.604 | -0.089 |
| HNO2 | 1.816e-026 | 1.816e-026 | -25.741 | -25.741 | 0.000 |
| FeNO2+2 | 0.000e+000 | 0.000e+000 | -49.602 | -49.934 | -0.332 |
| N(5) | 7.909e-003 | | | | |
| NO3- | 7.822e-003 | 6.374e-003 | -2.107 | -2.196 | -0.089 |
| CaNO3+ | 8.729e-005 | 7.197e-005 | -4.059 | -4.143 | -0.084 |
| HNO3 | 9.037e-017 | 9.037e-017 | -16.044 | -16.044 | 0.000 |
| FeNO3+2 | 4.527e-038 | 2.110e-038 | -37.344 | -37.676 | -0.332 |
| Na | 1.802e-002 | | | | |
| Na+ | 1.764e-002 | 1.454e-002 | -1.753 | -1.837 | -0.084 |
| NaSO4- | 3.247e-004 | 2.677e-004 | -3.489 | -3.572 | -0.084 |
| NaOH | 3.280e-005 | 3.280e-005 | -4.484 | -4.484 | 0.000 |
| NaCl | 1.446e-005 | 1.446e-005 | -4.840 | -4.840 | 0.000 |
| NaHSiO3 | 6.497e-006 | 6.497e-006 | -5.187 | -5.187 | 0.000 |
| NaAlO2 | 1.683e-006 | 1.683e-006 | -5.774 | -5.774 | 0.000 |
| NaCO3- | 1.225e-007 | 1.010e-007 | -6.912 | -6.996 | -0.084 |
| NaHCO3 | 3.703e-010 | 3.703e-010 | -9.431 | -9.431 | 0.000 |
| O(0) | 3.046e-003 | | | | |
| O2 | 1.523e-003 | 1.541e-003 | -2.817 | -2.812 | 0.005 |
| S(-2) | 0.000e+000 | | | | |
| HS- | 0.000e+000 | 0.000e+000 | -152.857 | -152.943 | -0.086 |
| S-2 | 0.000e+000 | 0.000e+000 | -153.384 | -153.707 | -0.323 |
| H2S | 0.000e+000 | 0.000e+000 | -158.255 | -158.255 | 0.000 |

```
  S2-2              0.000e+000  0.000e+000  -272.374  -272.715    -0.341
  S3-2              0.000e+000  0.000e+000  -391.418  -391.759    -0.341
  S4-2              0.000e+000  0.000e+000  -510.694  -511.035    -0.341
  S5-2              0.000e+000  0.000e+000  -630.196  -630.536    -0.341
S(2)         0.000e+000
  S2O3-2            0.000e+000  0.000e+000  -162.741  -163.082    -0.341
  HS2O3-            0.000e+000  0.000e+000  -174.447  -174.530    -0.084
S(3)         0.000e+000
  S2O4-2            0.000e+000  0.000e+000  -148.406  -148.729    -0.323
S(4)         0.000e+000
  SO3-2             0.000e+000  0.000e+000   -49.063   -49.395    -0.332
  HSO3-             0.000e+000  0.000e+000   -54.595   -54.679    -0.084
  H2SO3             0.000e+000  0.000e+000   -65.107   -65.107     0.000
  SO2               0.000e+000  0.000e+000   -65.360   -65.360     0.000
  S2O6-2            0.000e+000  0.000e+000   -81.822   -82.162    -0.341
  S3O6-2            0.000e+000  0.000e+000  -203.395  -203.736    -0.341
  S4O6-2            0.000e+000  0.000e+000  -308.703  -309.044    -0.341
  S5O6-2            0.000e+000  0.000e+000  -443.517  -443.858    -0.341
S(5)         0.000e+000
  S2O5-2            0.000e+000  0.000e+000  -113.827  -114.167    -0.341
S(6)         7.308e-003
  SO4-2             6.107e-003  2.786e-003    -2.214    -2.555    -0.341
  CaSO4             8.370e-004  8.370e-004    -3.077    -3.077     0.000
  NaSO4-            3.247e-004  2.677e-004    -3.489    -3.572    -0.084
  KSO4-             3.939e-005  3.247e-005    -4.405    -4.488    -0.084
  MgSO4             6.254e-009  6.254e-009    -8.204    -8.204     0.000
  HSO4-             8.879e-014  7.321e-014   -13.052   -13.135    -0.084
  LiSO4-            1.561e-015  1.287e-015   -14.806   -14.890    -0.084
  KHSO4             6.799e-018  6.799e-018   -17.168   -17.168     0.000
  AlSO4+            3.289e-029  2.712e-029   -28.483   -28.567    -0.084
  H2SO4             3.153e-029  3.153e-029   -28.501   -28.501     0.000
  Al(SO4)2-         7.113e-030  5.865e-030   -29.148   -29.232    -0.084
  FeSO4             1.823e-033  1.823e-033   -32.739   -32.739     0.000
  FeSO4+            7.405e-038  6.105e-038   -37.130   -37.214    -0.084
  Fe(SO4)2-         5.095e-039  4.201e-039   -38.293   -38.377    -0.084
  NH4SO4-           0.000e+000  0.000e+000   -87.439   -87.523    -0.084
S(7)         0.000e+000
  S2O8-2            0.000e+000  0.000e+000   -54.738   -55.079    -0.341
S(8)         3.548e-035
  HSO5-             3.548e-035  2.925e-035   -34.450   -34.534    -0.084
Si           2.272e-005
  HSiO3-            9.462e-006  7.801e-006    -5.024    -5.108    -0.084
  H2SiO4-2          6.733e-006  3.071e-006    -5.172    -5.513    -0.341
  NaHSiO3           6.497e-006  6.497e-006    -5.187    -5.187     0.000
  SiO2              3.334e-008  3.334e-008    -7.477    -7.477     0.000
  H4(H2SiO4)4-4     2.333e-015  9.969e-017   -14.632   -16.001    -1.369
  H6(H2SiO4)4-2     5.179e-019  2.363e-019   -18.286   -18.627    -0.341
```

## File 9. Degraded Cement, Minimum Ion Content, No Rebar

*INPUT FILE*

```
SOLUTION 1
    temp      15
    pH        7.5 charge
    pe        4
    redox     pe
    units     mmol/kgw
    density   1
    Alkalinity 0
    Cl(-1)    0
    Li        1e-010
```

```
   Al       1e-010
   Ca       0.6
   Mg       0.3
   Na       1.3
   K        0
   S(6)     0.3
   N(5)     0
   C(4)     1.4
   Br(-1)   0
   Si       0.01
   -water   1 # kg

GAS_PHASE 1
   -fixed_pressure
   -pressure 1
   -volume 1000
   -temperature 25
   CO2(g)   0.056
   O2(g)    0.18
EQUILIBRIUM_PHASES 1
   Brucite   0 1.39
   Calcite   0 9.5
   Gibbsite  0 0.001
   goethite  0 1e-005
   SiO2(am)  0 4
   CSH(0.25) 0 12
   Ca(OH)2*(CSH(1.5)) 0 0.01
SAVE solution 1-1
END
```

*SAMPLE OUTPUT, INITIAL CONDITION (FILE 9)*

```
 -------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 1.

-----------------------------Solution composition------------------------------

      Elements           Molality       Moles

      Al              1.000e-013  1.000e-013
      C(4)             1.400e-003  1.400e-003
      Ca               6.000e-004  6.000e-004
      Li              1.000e-013  1.000e-013
      Mg               3.000e-004  3.000e-004
      Na               1.300e-003  1.300e-003
      S(6)             3.000e-004  3.000e-004
      Si              1.000e-005  1.000e-005

----------------------------Description of solution----------------------------

                                pH  =  10.498      Charge balance
                                pe  =   4.000
                       Activity of water  =   1.000
                          Ionic strength  =  3.912e-003
                       Mass of water (kg)  =  1.000e+000
                  Total alkalinity (eq/kg)  =  2.500e-003
                       Total CO2 (mol/kg)  =  1.400e-003
                     Temperature (deg C)  =  15.000
                  Electrical balance (eq)  = -8.477e-013
```

```
Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                        Iterations  =   8
                          Total H  = 1.110513e+002
                          Total O  = 5.553090e+001
```

*SAMPLE OUTPUT, FINAL TIME STEP (FILE 9)*

```
-----------------------------------------
Beginning of batch-reaction calculations.
-----------------------------------------

Reaction step 1.

WARNING: Maximum iterations exceeded, 100

WARNING: Numerical method failed with this set of convergence parameters.

WARNING: Trying smaller step size, pe step size 10, 5 ...

WARNING: Maximum iterations exceeded, 200

WARNING: Numerical method failed with this set of convergence parameters.

WARNING: Trying reduced tolerance 1e-016 ...

Using solution 1.
Using pure phase assemblage 1.
Using gas phase 1.

-----------------------------------Gas phase----------------------------------


Total pressure:   1.0000   atmospheres
   Gas volume:  1.74e+002 liters

                                        Moles in gas
                                  ---------------------------------
Component              log P          P     Initial       Final       Delta

CO2(g)                  -8.09  8.188e-009  2.289e+000  6.022e-008 -2.289e+000
O2(g)                   -0.00  1.000e+000  7.357e+000  7.356e+000 -1.602e-003

-------------------------------Phase assemblage-------------------------------

                                        Moles in assemblage
Phase                SI log IAP  log KT      Initial       Final       Delta

Brucite             -0.00   16.96   16.96   1.390e+000  1.390e+000  1.155e-004
Ca(OH)2*(CSH(1.5))  -4.44   17.83   22.28   1.000e-002           0 -1.000e-002
Calcite             -0.00    1.98    1.98   9.500e+000  1.179e+001  2.290e+000
CSH(0.25)            0.00   14.96   14.96   1.200e+001  9.719e+000 -2.281e+000
Gibbsite            -0.00    8.36    8.36   1.000e-003  9.928e-004 -7.236e-006
Goethite            -0.00    0.91    0.91   1.000e-005  1.000e-005  3.030e-011
SiO2(am)             0.00   -2.87   -2.87   4.000e+000  6.276e+000  2.276e+000

-----------------------------Solution composition-----------------------------

      Elements           Molality       Moles

      Al              6.949e-006  7.236e-006
      C               1.594e-005  1.660e-005
      Ca              1.324e-003  1.379e-003
```

```
      Fe            6.693e-011  6.969e-011
      Li            9.604e-014  1.000e-013
      Mg            1.772e-004  1.845e-004
      Na            1.249e-003  1.300e-003
      S             2.881e-004  3.000e-004
      Si            4.979e-003  5.184e-003

----------Description of solution----------

                          pH  =  10.428     Charge balance
                          pe  =  11.099     Adjusted to redox equilibrium
                Activity of water  =  1.000
                  Ionic strength  =  5.864e-003
                Mass of water (kg)  =  1.041e+000
           Total alkalinity (eq/kg)  =  3.696e-003
              Total CO2 (mol/kg)  =  1.594e-005
             Temperature (deg C)  =  15.000
           Electrical balance (eq)  =  1.516e-012
Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  0.00
                    Iterations  =  93
                      Total H  = 1.156331e+002
                      Total O  = 5.783330e+001

----------Distribution of species----------

                                    Log      Log       Log
  Species          Molality    Activity  Molality  Activity     Gamma

  OH-            1.280e-004  1.180e-004    -3.893    -3.928    -0.035
  H+             4.007e-011  3.729e-011   -10.397   -10.428    -0.031
  H2O            5.553e+001  9.998e-001     1.744    -0.000     0.000
Al          6.949e-006
  AlO2-          6.947e-006  6.411e-006    -5.158    -5.193    -0.035
  HAlO2          1.165e-009  1.165e-009    -8.934    -8.934     0.000
  NaAlO2         1.066e-009  1.066e-009    -8.972    -8.972     0.000
  Al(OH)2+       6.180e-014  5.703e-014   -13.209   -13.244    -0.035
  AlOH+2         2.490e-018  1.809e-018   -17.604   -17.742    -0.139
  Al+3           2.308e-023  1.202e-023   -22.637   -22.920    -0.283
  AlSO4+         2.492e-024  2.299e-024   -23.604   -23.638    -0.035
  Al(SO4)2-      3.617e-026  3.338e-026   -25.442   -25.477    -0.035
  Al2(OH)2+4     7.395e-033  2.119e-033   -32.131   -32.674    -0.543
  Al3(OH)4+5     0.000e+000  0.000e+000   -40.088   -40.928    -0.839
  Al13O4(OH)24+7 0.000e+000  0.000e+000   -61.341   -62.986    -1.645
C(-2)       0.000e+000
  C2H4           0.000e+000  0.000e+000  -286.907  -286.907     0.000
C(-3)       0.000e+000
  C2H6           0.000e+000  0.000e+000  -258.758  -258.758     0.000
C(-4)       0.000e+000
  CH4            0.000e+000  0.000e+000  -159.557  -159.557     0.000
C(2)        0.000e+000
  CO             0.000e+000  0.000e+000   -57.791   -57.791     0.000
C(4)        1.594e-005
  CaCO3          6.322e-006  6.322e-006    -5.199    -5.199     0.000
  CO3-2          5.019e-006  3.648e-006    -5.299    -5.438    -0.139
  HCO3-          4.098e-006  3.782e-006    -5.387    -5.422    -0.035
  MgCO3          4.277e-007  4.277e-007    -6.369    -6.369     0.000
  CaHCO3+        4.536e-008  4.186e-008    -7.343    -7.378    -0.035
  NaCO3-         1.786e-008  1.648e-008    -7.748    -7.783    -0.035
  NaHCO3         6.536e-009  6.536e-009    -8.185    -8.185     0.000
  MgHCO3+        5.951e-009  5.492e-009    -8.225    -8.260    -0.035
  CO2            3.789e-010  3.794e-010    -9.422    -9.421     0.001
  FeCO3+         2.394e-026  2.209e-026   -25.621   -25.656    -0.035
```

| | | | | | |
|---|---|---|---|---|---|
| FeCO3 | 1.233e-029 | 1.233e-029 | -28.909 | -28.909 | 0.000 |
| FeHCO3+ | 1.038e-031 | 9.578e-032 | -30.984 | -31.019 | -0.035 |
| Ca | 1.324e-003 | | | | |
| Ca+2 | 1.290e-003 | 9.476e-004 | -2.889 | -3.023 | -0.134 |
| CaSO4 | 2.363e-005 | 2.363e-005 | -4.626 | -4.626 | 0.000 |
| CaCO3 | 6.322e-006 | 6.322e-006 | -5.199 | -5.199 | 0.000 |
| CaOH+ | 3.889e-006 | 3.589e-006 | -5.410 | -5.445 | -0.035 |
| CaHCO3+ | 4.536e-008 | 4.186e-008 | -7.343 | -7.378 | -0.035 |
| Fe(2) | 7.109e-028 | | | | |
| FeOH+ | 4.434e-028 | 4.092e-028 | -27.353 | -27.388 | -0.035 |
| Fe(OH)3- | 1.008e-028 | 9.303e-029 | -27.997 | -28.031 | -0.035 |
| Fe(OH)2 | 8.715e-029 | 8.715e-029 | -28.060 | -28.060 | 0.000 |
| Fe+2 | 6.571e-029 | 4.826e-029 | -28.182 | -28.316 | -0.134 |
| FeCO3 | 1.233e-029 | 1.233e-029 | -28.909 | -28.909 | 0.000 |
| FeSO4 | 1.430e-030 | 1.430e-030 | -29.845 | -29.845 | 0.000 |
| FeHCO3+ | 1.038e-031 | 9.578e-032 | -30.984 | -31.019 | -0.035 |
| Fe(OH)4-2 | 3.445e-033 | 2.494e-033 | -32.463 | -32.603 | -0.140 |
| Fe(3) | 6.693e-011 | | | | |
| Fe(OH)4- | 5.886e-011 | 5.432e-011 | -10.230 | -10.265 | -0.035 |
| Fe(OH)3 | 8.065e-012 | 8.065e-012 | -11.093 | -11.093 | 0.000 |
| Fe(OH)2+ | 6.969e-016 | 6.431e-016 | -15.157 | -15.192 | -0.035 |
| FeOH+2 | 9.967e-023 | 7.243e-023 | -22.001 | -22.140 | -0.139 |
| FeCO3+ | 2.394e-026 | 2.209e-026 | -25.621 | -25.656 | -0.035 |
| Fe+3 | 8.035e-031 | 4.184e-031 | -30.095 | -30.378 | -0.283 |
| FeSO4+ | 5.615e-033 | 5.181e-033 | -32.251 | -32.286 | -0.035 |
| Fe(SO4)2- | 2.593e-035 | 2.393e-035 | -34.586 | -34.621 | -0.035 |
| Fe2(OH)2+4 | 0.000e+000 | 0.000e+000 | -42.307 | -42.850 | -0.543 |
| Fe3(OH)4+5 | 0.000e+000 | 0.000e+000 | -54.883 | -55.722 | -0.839 |
| H(0) | 0.000e+000 | | | | |
| H2 | 0.000e+000 | 0.000e+000 | -46.364 | -46.363 | 0.001 |
| Li | 9.604e-014 | | | | |
| Li+ | 9.588e-014 | 8.879e-014 | -13.018 | -13.052 | -0.033 |
| LiSO4- | 1.060e-016 | 9.778e-017 | -15.975 | -16.010 | -0.035 |
| LiOH | 5.454e-017 | 5.454e-017 | -16.263 | -16.263 | 0.000 |
| Mg | 1.772e-004 | | | | |
| Mg+2 | 1.719e-004 | 1.279e-004 | -3.765 | -3.893 | -0.128 |
| MgSO4 | 4.905e-006 | 4.905e-006 | -5.309 | -5.309 | 0.000 |
| MgCO3 | 4.277e-007 | 4.277e-007 | -6.369 | -6.369 | 0.000 |
| MgHCO3+ | 5.951e-009 | 5.492e-009 | -8.225 | -8.260 | -0.035 |
| Mg4(OH)4+4 | 8.578e-014 | 2.457e-014 | -13.067 | -13.610 | -0.543 |
| Na | 1.249e-003 | | | | |
| Na+ | 1.082e-003 | 9.981e-004 | -2.966 | -3.001 | -0.035 |
| NaHSiO3 | 1.656e-004 | 1.656e-004 | -3.781 | -3.781 | 0.000 |
| NaSO4- | 1.336e-006 | 1.233e-006 | -5.874 | -5.909 | -0.035 |
| NaOH | 2.082e-008 | 2.082e-008 | -7.681 | -7.681 | 0.000 |
| NaCO3- | 1.786e-008 | 1.648e-008 | -7.748 | -7.783 | -0.035 |
| NaHCO3 | 6.536e-009 | 6.536e-009 | -8.185 | -8.185 | 0.000 |
| NaAlO2 | 1.066e-009 | 1.066e-009 | -8.972 | -8.972 | 0.000 |
| O(0) | 3.077e-003 | | | | |
| O2 | 1.539e-003 | 1.541e-003 | -2.813 | -2.812 | 0.001 |
| S(-2) | 0.000e+000 | | | | |
| HS- | 0.000e+000 | 0.000e+000 | -152.047 | -152.082 | -0.035 |
| S-2 | 0.000e+000 | 0.000e+000 | -154.743 | -154.880 | -0.137 |
| H2S | 0.000e+000 | 0.000e+000 | -155.360 | -155.360 | 0.000 |
| S2-2 | 0.000e+000 | 0.000e+000 | -270.853 | -270.993 | -0.140 |
| S3-2 | 0.000e+000 | 0.000e+000 | -387.002 | -387.142 | -0.140 |
| S4-2 | 0.000e+000 | 0.000e+000 | -503.383 | -503.523 | -0.140 |
| S5-2 | 0.000e+000 | 0.000e+000 | -619.990 | -620.130 | -0.140 |
| S(2) | 0.000e+000 | | | | |
| S2O3-2 | 0.000e+000 | 0.000e+000 | -161.220 | -161.360 | -0.140 |
| HS2O3- | 0.000e+000 | 0.000e+000 | -170.740 | -170.774 | -0.035 |
| S(3) | 0.000e+000 | | | | |

```
  S2O4-2             0.000e+000  0.000e+000  -146.870  -147.007    -0.137
S(4)          0.000e+000
  SO3-2              0.000e+000  0.000e+000   -50.429   -50.568    -0.139
  HSO3-              0.000e+000  0.000e+000   -53.783   -53.818    -0.035
  H2SO3              0.000e+000  0.000e+000   -62.212   -62.212     0.000
  SO2                0.000e+000  0.000e+000   -62.465   -62.465     0.000
  S2O6-2             0.000e+000  0.000e+000   -80.300   -80.441    -0.140
  S3O6-2             0.000e+000  0.000e+000  -198.979  -199.119    -0.140
  S4O6-2             0.000e+000  0.000e+000  -301.392  -301.533    -0.140
  S5O6-2             0.000e+000  0.000e+000  -433.311  -433.451    -0.140
S(5)          0.000e+000
  S2O5-2             0.000e+000  0.000e+000  -112.305  -112.446    -0.140
S(6)          2.881e-004
  SO4-2              2.582e-004  1.870e-004    -3.588    -3.728    -0.140
  CaSO4              2.363e-005  2.363e-005    -4.626    -4.626     0.000
  MgSO4              4.905e-006  4.905e-006    -5.309    -5.309     0.000
  NaSO4-             1.336e-006  1.233e-006    -5.874    -5.909    -0.035
  HSO4-              5.762e-013  5.317e-013   -12.239   -12.274    -0.035
  LiSO4-             1.060e-016  9.778e-017   -15.975   -16.010    -0.035
  AlSO4+             2.492e-024  2.299e-024   -23.604   -23.638    -0.035
  Al(SO4)2-          3.617e-026  3.338e-026   -25.442   -25.477    -0.035
  H2SO4              2.478e-026  2.478e-026   -25.606   -25.606     0.000
  FeSO4              1.430e-030  1.430e-030   -29.845   -29.845     0.000
  FeSO4+             5.615e-033  5.181e-033   -32.251   -32.286    -0.035
  Fe(SO4)2-          2.593e-035  2.393e-035   -34.586   -34.621    -0.035
S(7)          0.000e+000
  S2O8-2             0.000e+000  0.000e+000   -53.217   -53.357    -0.140
S(8)          2.302e-034
  HSO5-              2.302e-034  2.125e-034   -33.638   -33.673    -0.035
Si            4.979e-003
  HSiO3-             3.140e-003  2.898e-003    -2.503    -2.538    -0.035
  SiO2               1.339e-003  1.339e-003    -2.873    -2.873     0.000
  NaHSiO3            1.656e-004  1.656e-004    -3.781    -3.781     0.000
  H6(H2SiO4)4-2      7.299e-005  5.285e-005    -4.137    -4.277    -0.140
  H2SiO4-2           1.457e-005  1.055e-005    -4.836    -4.977    -0.140
  H4(H2SiO4)4-4      6.940e-006  1.905e-006    -5.159    -5.720    -0.561
```

## File 10. Degraded Cement, Maximum Ion Content, No Rebar

*INPUT FILE*

```
SOLUTION 1
    temp      15
    pH        7.5 charge
    pe        4
    redox     pe
    units     mmol/kgw
    density   1
    Alkalinity 0
    Cl(-1)    7.5
    Li        1e-010
    Al        1e-010
    Ca        3.1
    Mg        5
    Na        18
    K         1.9
    S(6)      7.3
    N(5)      7.9
    C(4)      21.8
    Br(-1)    0
    Si        0.01
    -water    1 # kg
```

```
GAS_PHASE 1
   -fixed_pressure
   -pressure 1
   -volume 1000
   -temperature 25
   CO2(g)    0.056
   O2(g)     0.18
EQUILIBRIUM_PHASES 1
   Brucite   0 1.39
   Calcite   0 9.5
   Gibbsite  0 0.001
   goethite  0 1e-005
   SiO2(am)  0 4
   CSH(0.25) 0 12
   Ca(OH)2*(CSH(1.5)) 0 0.01
SAVE solution 1-1
END
```

*SAMPLE OUTPUT, INITIAL CONDITION (FILE 10)*

```
 -------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 1.

-----------------------------Solution composition------------------------------

      Elements           Molality       Moles

      Al              1.000e-013  1.000e-013
      C(4)             2.180e-002  2.180e-002
      Ca               3.100e-003  3.100e-003
      Cl(-1)           7.500e-003  7.500e-003
      K               1.900e-003  1.900e-003
      Li              1.000e-013  1.000e-013
      Mg               5.000e-003  5.000e-003
      N(5)             7.900e-003  7.900e-003
      Na               1.800e-002  1.800e-002
      S(6)             7.300e-003  7.300e-003
      Si              1.000e-005  1.000e-005

----------------------------Description of solution----------------------------

                                pH  =   5.909      Charge balance
                                pe  =   4.000
                       Activity of water  =   0.999
                          Ionic strength  =  4.415e-002
                       Mass of water (kg)  =  1.000e+000
                  Total alkalinity (eq/kg)  =  6.100e-003
                       Total CO2 (mol/kg)  =  2.180e-002
                     Temperature (deg C)  =  15.000
                  Electrical balance (eq)  = -1.388e-017
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                            Iterations  =   8
                              Total H  = 1.110568e+002
                              Total O  = 5.562795e+001
```

*SAMPLE OUTPUT, FINAL TIME STEP (FILE 10)*

```
-------------------------------------------
```

Beginning of batch-reaction calculations.
---

Reaction step 1.

Using solution 1.
Using pure phase assemblage 1.
Using gas phase 1.

----------Gas phase----------

Total pressure: 1.0000 atmospheres
Gas volume: 1.74e+002 liters

| | | | Moles in gas | | |
|---|---|---|---|---|---|
| Component | log P | P | Initial | Final | Delta |
| CO2(g) | -8.09 | 8.182e-009 | 2.289e+000 | 6.018e-008 | -2.289e+000 |
| O2(g) | -0.00 | 1.000e+000 | 7.357e+000 | 7.356e+000 | -1.589e-003 |

----------Phase assemblage----------

| | | | Moles in assemblage | | |
|---|---|---|---|---|---|
| Phase | SI log IAP | log KT | Initial | Final | Delta |
| Brucite | 0.00 | 16.96 | 16.96 | 1.390e+000 | 1.394e+000 | 4.155e-003 |
| Ca(OH)2*(CSH(1.5)) | -4.44 | 17.83 | 22.28 | 1.000e-002 | 0 | -1.000e-002 |
| Calcite | -0.00 | 1.98 | 1.98 | 9.500e+000 | 1.181e+001 | 2.311e+000 |
| CSH(0.25) | 0.00 | 14.96 | 14.96 | 1.200e+001 | 9.696e+000 | -2.304e+000 |
| Gibbsite | 0.00 | 8.36 | 8.36 | 1.000e-003 | 9.951e-004 | -4.925e-006 |
| Goethite | 0.00 | 0.91 | 0.91 | 1.000e-005 | 1.000e-005 | -4.995e-011 |
| SiO2(am) | 0.00 | -2.87 | -2.87 | 4.000e+000 | 6.299e+000 | 2.299e+000 |

----------Solution composition----------

| Elements | Molality | Moles |
|---|---|---|
| Al | 4.728e-006 | 4.925e-006 |
| C | 1.257e-005 | 1.309e-005 |
| Ca | 5.888e-003 | 6.133e-003 |
| Cl | 7.200e-003 | 7.500e-003 |
| Fe | 4.795e-011 | 4.995e-011 |
| K | 1.824e-003 | 1.900e-003 |
| Li | 9.601e-014 | 1.000e-013 |
| Mg | 8.112e-004 | 8.450e-004 |
| N | 7.584e-003 | 7.900e-003 |
| Na | 1.728e-002 | 1.800e-002 |
| S | 7.008e-003 | 7.300e-003 |
| Si | 4.994e-003 | 5.202e-003 |

----------Description of solution----------

pH = 10.217 Charge balance
pe = 11.310 Adjusted to redox equilibrium
Activity of water = 0.999
Ionic strength = 3.972e-002
Mass of water (kg) = 1.042e+000
Total alkalinity (eq/kg) = 3.716e-003
Total CO2 (mol/kg) = 1.257e-005
Temperature (deg C) = 15.000

Electrical balance (eq) = -6.939e-018
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.00
Iterations = 54
Total H = 1.156759e+002
Total O = 5.790637e+001

----------Distribution of species----------

| Species | Molality | Log Activity | Log Molality | Log Activity | Gamma |
|---|---|---|---|---|---|
| OH- | 8.713e-005 | 7.243e-005 | -4.060 | -4.140 | -0.080 |
| H+ | 6.997e-011 | 6.070e-011 | -10.155 | -10.217 | -0.062 |
| H2O | 5.553e+001 | 9.991e-001 | 1.744 | -0.000 | 0.000 |
| Al | 4.728e-006 | | | | |
| AlO2- | 4.718e-006 | 3.941e-006 | -5.326 | -5.404 | -0.078 |
| NaAlO2 | 8.590e-009 | 8.590e-009 | -8.066 | -8.066 | 0.000 |
| HAlO2 | 1.166e-009 | 1.166e-009 | -8.933 | -8.933 | 0.000 |
| Al(OH)2+ | 1.112e-013 | 9.290e-014 | -12.954 | -13.032 | -0.078 |
| AlOH+2 | 9.785e-018 | 4.801e-018 | -17.009 | -17.319 | -0.309 |
| Al+3 | 1.923e-022 | 5.194e-023 | -21.716 | -22.285 | -0.568 |
| AlSO4+ | 1.716e-022 | 1.433e-022 | -21.765 | -21.844 | -0.078 |
| Al(SO4)2- | 3.593e-023 | 3.001e-023 | -22.445 | -22.523 | -0.078 |
| Al2(OH)2+4 | 2.268e-031 | 1.492e-032 | -30.644 | -31.826 | -1.182 |
| Al3(OH)4+5 | 8.636e-039 | 1.355e-040 | -38.064 | -39.868 | -1.804 |
| Al13O4(OH)24+7 | 0.000e+000 | 0.000e+000 | -57.963 | -61.501 | -3.538 |
| C(-2) | 0.000e+000 | | | | |
| C2H4 | 0.000e+000 | 0.000e+000 | -286.908 | -286.908 | 0.000 |
| C(-3) | 0.000e+000 | | | | |
| C2H6 | 0.000e+000 | 0.000e+000 | -258.759 | -258.759 | 0.000 |
| C(-4) | 0.000e+000 | | | | |
| CH4 | 0.000e+000 | 0.000e+000 | -159.558 | -159.558 | 0.000 |
| C(2) | 0.000e+000 | | | | |
| CO | 0.000e+000 | 0.000e+000 | -57.791 | -57.791 | 0.000 |
| C(4) | 1.257e-005 | | | | |
| CaCO3 | 6.322e-006 | 6.322e-006 | -5.199 | -5.199 | 0.000 |
| CO3-2 | 2.802e-006 | 1.375e-006 | -5.553 | -5.862 | -0.309 |
| HCO3- | 2.777e-006 | 2.320e-006 | -5.556 | -5.635 | -0.078 |
| MgCO3 | 4.277e-007 | 4.277e-007 | -6.369 | -6.369 | 0.000 |
| NaCO3- | 9.745e-008 | 8.140e-008 | -7.011 | -7.089 | -0.078 |
| CaHCO3+ | 8.158e-008 | 6.814e-008 | -7.088 | -7.167 | -0.078 |
| NaHCO3 | 5.254e-008 | 5.254e-008 | -7.280 | -7.280 | 0.000 |
| MgHCO3+ | 1.070e-008 | 8.939e-009 | -7.971 | -8.049 | -0.078 |
| CO2 | 3.755e-010 | 3.791e-010 | -9.425 | -9.421 | 0.004 |
| FeCO3+ | 4.305e-026 | 3.596e-026 | -25.366 | -25.444 | -0.078 |
| FeCO3 | 1.232e-029 | 1.232e-029 | -28.909 | -28.909 | 0.000 |
| FeHCO3+ | 1.866e-031 | 1.559e-031 | -30.729 | -30.807 | -0.078 |
| Ca | 5.888e-003 | | | | |
| Ca+2 | 4.873e-003 | 2.514e-003 | -2.312 | -2.600 | -0.287 |
| CaSO4 | 9.045e-004 | 9.045e-004 | -3.044 | -3.044 | 0.000 |
| CaNO3+ | 9.346e-005 | 7.807e-005 | -4.029 | -4.108 | -0.078 |
| CaOH+ | 6.999e-006 | 5.846e-006 | -5.155 | -5.233 | -0.078 |
| CaCO3 | 6.322e-006 | 6.322e-006 | -5.199 | -5.199 | 0.000 |
| CaCl+ | 3.693e-006 | 3.085e-006 | -5.433 | -5.511 | -0.078 |
| CaHCO3+ | 8.158e-008 | 6.814e-008 | -7.088 | -7.167 | -0.078 |
| CaCl2 | 2.402e-008 | 2.402e-008 | -7.619 | -7.619 | 0.000 |
| Cl(-1) | 7.200e-003 | | | | |
| Cl- | 7.182e-003 | 5.939e-003 | -2.144 | -2.226 | -0.082 |
| NaCl | 1.265e-005 | 1.265e-005 | -4.898 | -4.898 | 0.000 |
| CaCl+ | 3.693e-006 | 3.085e-006 | -5.433 | -5.511 | -0.078 |
| MgCl+ | 1.912e-006 | 1.597e-006 | -5.718 | -5.797 | -0.078 |
| KCl | 2.395e-007 | 2.395e-007 | -6.621 | -6.621 | 0.000 |

| | | | | | |
|---|---|---|---|---|---|
| CaCl2 | 2.402e-008 | 2.402e-008 | -7.619 | -7.619 | 0.000 |
| HCl | 7.945e-014 | 7.945e-014 | -13.100 | -13.100 | 0.000 |
| LiCl | 1.456e-017 | 1.456e-017 | -16.837 | -16.837 | 0.000 |
| FeCl+ | 6.372e-031 | 5.323e-031 | -30.196 | -30.274 | -0.078 |
| FeCl2+ | 1.029e-032 | 8.600e-033 | -31.987 | -32.066 | -0.078 |
| FeCl+2 | 2.181e-033 | 1.070e-033 | -32.661 | -32.971 | -0.309 |
| FeCl2 | 1.613e-035 | 1.613e-035 | -34.792 | -34.792 | 0.000 |
| FeCl4-2 | 3.367e-039 | 1.622e-039 | -38.473 | -38.790 | -0.317 |
| FeCl4- | 4.366e-040 | 3.647e-040 | -39.360 | -39.438 | -0.078 |
| Cl(1) | 8.564e-020 | | | | |
| ClO- | 8.548e-020 | 7.140e-020 | -19.068 | -19.146 | -0.078 |
| HClO | 1.607e-022 | 1.607e-022 | -21.794 | -21.794 | 0.000 |
| Cl(3) | 1.705e-029 | | | | |
| ClO2- | 1.705e-029 | 1.424e-029 | -28.768 | -28.847 | -0.078 |
| HClO2 | 1.278e-036 | 1.278e-036 | -35.894 | -35.894 | 0.000 |
| Cl(5) | 7.313e-025 | | | | |
| ClO3- | 7.313e-025 | 6.079e-025 | -24.136 | -24.216 | -0.080 |
| Cl(7) | 1.309e-024 | | | | |
| ClO4- | 1.309e-024 | 1.088e-024 | -23.883 | -23.963 | -0.080 |
| Fe(2) | 1.269e-027 | | | | |
| FeOH+ | 7.976e-028 | 6.663e-028 | -27.098 | -27.176 | -0.078 |
| Fe+2 | 2.481e-028 | 1.280e-028 | -27.605 | -27.893 | -0.287 |
| Fe(OH)2 | 8.712e-029 | 8.712e-029 | -28.060 | -28.060 | 0.000 |
| Fe(OH)3- | 6.834e-029 | 5.709e-029 | -28.165 | -28.243 | -0.078 |
| FeSO4 | 5.472e-029 | 5.472e-029 | -28.262 | -28.262 | 0.000 |
| FeCO3 | 1.232e-029 | 1.232e-029 | -28.909 | -28.909 | 0.000 |
| FeCl+ | 6.372e-031 | 5.323e-031 | -30.196 | -30.274 | -0.078 |
| FeHCO3+ | 1.866e-031 | 1.559e-031 | -30.729 | -30.807 | -0.078 |
| Fe(OH)4-2 | 1.951e-033 | 9.397e-034 | -32.710 | -33.027 | -0.317 |
| FeCl2 | 1.613e-035 | 1.613e-035 | -34.792 | -34.792 | 0.000 |
| FeCl4-2 | 3.367e-039 | 1.622e-039 | -38.473 | -38.790 | -0.317 |
| Fe(3) | 4.795e-011 | | | | |
| Fe(OH)4- | 3.989e-011 | 3.332e-011 | -10.399 | -10.477 | -0.078 |
| Fe(OH)3 | 8.060e-012 | 8.060e-012 | -11.094 | -11.094 | 0.000 |
| Fe(OH)2+ | 1.253e-015 | 1.047e-015 | -14.902 | -14.980 | -0.078 |
| FeOH+2 | 3.915e-022 | 1.921e-022 | -21.407 | -21.717 | -0.309 |
| FeCO3+ | 4.305e-026 | 3.596e-026 | -25.366 | -25.444 | -0.078 |
| Fe+3 | 6.690e-030 | 1.807e-030 | -29.175 | -29.743 | -0.568 |
| FeSO4+ | 3.864e-031 | 3.228e-031 | -30.413 | -30.491 | -0.078 |
| FeNO3+2 | 2.282e-031 | 1.120e-031 | -30.642 | -30.951 | -0.309 |
| Fe(SO4)2- | 2.574e-032 | 2.150e-032 | -31.589 | -31.667 | -0.078 |
| FeCl2+ | 1.029e-032 | 8.600e-033 | -31.987 | -32.066 | -0.078 |
| FeCl+2 | 2.181e-033 | 1.070e-033 | -32.661 | -32.971 | -0.309 |
| FeCl4- | 4.366e-040 | 3.647e-040 | -39.360 | -39.438 | -0.078 |
| Fe2(OH)2+4 | 0.000e+000 | 0.000e+000 | -40.821 | -42.003 | -1.182 |
| FeNO2+2 | 0.000e+000 | 0.000e+000 | -42.900 | -43.209 | -0.309 |
| Fe3(OH)4+5 | 0.000e+000 | 0.000e+000 | -52.859 | -54.663 | -1.804 |
| H(0) | 0.000e+000 | | | | |
| H2 | 0.000e+000 | 0.000e+000 | -46.368 | -46.363 | 0.004 |
| K | 1.824e-003 | | | | |
| K+ | 1.787e-003 | 1.478e-003 | -2.748 | -2.830 | -0.082 |
| KSO4- | 3.694e-005 | 3.086e-005 | -4.432 | -4.511 | -0.078 |
| KCl | 2.395e-007 | 2.395e-007 | -6.621 | -6.621 | 0.000 |
| KOH | 8.434e-008 | 8.434e-008 | -7.074 | -7.074 | 0.000 |
| KHSO4 | 1.138e-015 | 1.138e-015 | -14.944 | -14.944 | 0.000 |
| Li | 9.601e-014 | | | | |
| Li+ | 9.443e-014 | 8.025e-014 | -13.025 | -13.096 | -0.071 |
| LiSO4- | 1.526e-015 | 1.275e-015 | -14.816 | -14.895 | -0.078 |
| LiOH | 3.026e-017 | 3.026e-017 | -16.519 | -16.519 | 0.000 |
| LiCl | 1.456e-017 | 1.456e-017 | -16.837 | -16.837 | 0.000 |
| Mg | 8.112e-004 | | | | |
| Mg+2 | 6.211e-004 | 3.393e-004 | -3.207 | -3.469 | -0.263 |

| | | | | | |
|---|---|---|---|---|---|
| MgSO4 | 1.877e-004 | 1.877e-004 | -3.726 | -3.726 | 0.000 |
| MgCl+ | 1.912e-006 | 1.597e-006 | -5.718 | -5.797 | -0.078 |
| MgCO3 | 4.277e-007 | 4.277e-007 | -6.369 | -6.369 | 0.000 |
| MgHCO3+ | 1.070e-008 | 8.939e-009 | -7.971 | -8.049 | -0.078 |
| Mg4(OH)4+4 | 2.631e-012 | 1.730e-013 | -11.580 | -12.762 | -1.182 |
| N(-03) | 0.000e+000 | | | | |
| N3- | 0.000e+000 | 0.000e+000 | -108.385 | -108.463 | -0.078 |
| HN3 | 0.000e+000 | 0.000e+000 | -113.885 | -113.885 | 0.000 |
| N(-3) | 0.000e+000 | | | | |
| NH3 | 0.000e+000 | 0.000e+000 | -71.211 | -71.211 | 0.000 |
| NH4+ | 0.000e+000 | 0.000e+000 | -71.789 | -71.873 | -0.085 |
| NH4SO4- | 0.000e+000 | 0.000e+000 | -82.979 | -83.057 | -0.078 |
| N(0) | 1.964e-026 | | | | |
| N2 | 9.822e-027 | 9.822e-027 | -26.008 | -26.008 | 0.000 |
| N(3) | 2.928e-017 | | | | |
| NO2- | 2.928e-017 | 2.421e-017 | -16.533 | -16.616 | -0.082 |
| HNO2 | 3.108e-024 | 3.108e-024 | -23.508 | -23.508 | 0.000 |
| FeNO2+2 | 0.000e+000 | 0.000e+000 | -42.900 | -43.209 | -0.309 |
| N(5) | 7.584e-003 | | | | |
| NO3- | 7.491e-003 | 6.195e-003 | -2.125 | -2.208 | -0.082 |
| CaNO3+ | 9.346e-005 | 7.807e-005 | -4.029 | -4.108 | -0.078 |
| HNO3 | 1.547e-014 | 1.547e-014 | -13.811 | -13.811 | 0.000 |
| FeNO3+2 | 2.282e-031 | 1.120e-031 | -30.642 | -30.951 | -0.309 |
| Na | 1.728e-002 | | | | |
| Na+ | 1.566e-002 | 1.308e-002 | -1.805 | -1.883 | -0.078 |
| NaHSiO3 | 1.332e-003 | 1.332e-003 | -2.875 | -2.875 | 0.000 |
| NaSO4- | 2.790e-004 | 2.331e-004 | -3.554 | -3.633 | -0.078 |
| NaCl | 1.265e-005 | 1.265e-005 | -4.898 | -4.898 | 0.000 |
| NaOH | 1.675e-007 | 1.675e-007 | -6.776 | -6.776 | 0.000 |
| NaCO3- | 9.745e-008 | 8.140e-008 | -7.011 | -7.089 | -0.078 |
| NaHCO3 | 5.254e-008 | 5.254e-008 | -7.280 | -7.280 | 0.000 |
| NaAlO2 | 8.590e-009 | 8.590e-009 | -8.066 | -8.066 | 0.000 |
| O(0) | 3.052e-003 | | | | |
| O2 | 1.526e-003 | 1.541e-003 | -2.816 | -2.812 | 0.004 |
| S(-2) | 0.000e+000 | | | | |
| HS- | 0.000e+000 | 0.000e+000 | -150.631 | -150.711 | -0.080 |
| S-2 | 0.000e+000 | 0.000e+000 | -153.420 | -153.721 | -0.302 |
| H2S | 0.000e+000 | 0.000e+000 | -153.777 | -153.777 | 0.000 |
| S2-2 | 0.000e+000 | 0.000e+000 | -267.934 | -268.251 | -0.317 |
| S3-2 | 0.000e+000 | 0.000e+000 | -382.501 | -382.818 | -0.317 |
| S4-2 | 0.000e+000 | 0.000e+000 | -497.299 | -497.616 | -0.317 |
| S5-2 | 0.000e+000 | 0.000e+000 | -612.323 | -612.641 | -0.317 |
| S(2) | 0.000e+000 | | | | |
| S2O3-2 | 0.000e+000 | 0.000e+000 | -158.301 | -158.618 | -0.317 |
| HS2O3- | 0.000e+000 | 0.000e+000 | -167.743 | -167.821 | -0.078 |
| S(3) | 0.000e+000 | | | | |
| S2O4-2 | 0.000e+000 | 0.000e+000 | -143.964 | -144.266 | -0.302 |
| S(4) | 0.000e+000 | | | | |
| SO3-2 | 0.000e+000 | 0.000e+000 | -49.100 | -49.409 | -0.309 |
| HSO3- | 0.000e+000 | 0.000e+000 | -52.369 | -52.447 | -0.078 |
| H2SO3 | 0.000e+000 | 0.000e+000 | -60.629 | -60.629 | 0.000 |
| SO2 | 0.000e+000 | 0.000e+000 | -60.882 | -60.882 | 0.000 |
| S2O6-2 | 0.000e+000 | 0.000e+000 | -77.382 | -77.699 | -0.317 |
| S3O6-2 | 0.000e+000 | 0.000e+000 | -194.478 | -194.795 | -0.317 |
| S4O6-2 | 0.000e+000 | 0.000e+000 | -295.308 | -295.626 | -0.317 |
| S5O6-2 | 0.000e+000 | 0.000e+000 | -425.645 | -425.962 | -0.317 |
| S(5) | 0.000e+000 | | | | |
| S2O5-2 | 0.000e+000 | 0.000e+000 | -109.387 | -109.704 | -0.317 |
| S(6) | 7.008e-003 | | | | |
| SO4-2 | 5.600e-003 | 2.697e-003 | -2.252 | -2.569 | -0.317 |
| CaSO4 | 9.045e-004 | 9.045e-004 | -3.044 | -3.044 | 0.000 |
| NaSO4- | 2.790e-004 | 2.331e-004 | -3.554 | -3.633 | -0.078 |

```
  MgSO4              1.877e-004  1.877e-004   -3.726   -3.726    0.000
  KSO4-              3.694e-005  3.086e-005   -4.432   -4.511   -0.078
  HSO4-              1.494e-011  1.248e-011  -10.826  -10.904   -0.078
  LiSO4-             1.526e-015  1.275e-015  -14.816  -14.895   -0.078
  KHSO4              1.138e-015  1.138e-015  -14.944  -14.944    0.000
  AlSO4+             1.716e-022  1.433e-022  -21.765  -21.844   -0.078
  Al(SO4)2-          3.593e-023  3.001e-023  -22.445  -22.523   -0.078
  H2SO4              9.470e-025  9.470e-025  -24.024  -24.024    0.000
  FeSO4              5.472e-029  5.472e-029  -28.262  -28.262    0.000
  FeSO4+             3.864e-031  3.228e-031  -30.413  -30.491   -0.078
  Fe(SO4)2-          2.574e-032  2.150e-032  -31.589  -31.667   -0.078
  NH4SO4-            0.000e+000  0.000e+000  -82.979  -83.057   -0.078
S(7)          0.000e+000
  S2O8-2             0.000e+000  0.000e+000  -50.298  -50.615   -0.317
S(8)          5.972e-033
  HSO5-              5.972e-033  4.989e-033  -32.224  -32.302   -0.078
Si            4.994e-003
  HSiO3-             2.130e-003  1.779e-003   -2.672   -2.750   -0.078
  SiO2               1.339e-003  1.339e-003   -2.873   -2.873    0.000
  NaHSiO3            1.332e-003  1.332e-003   -2.875   -2.875    0.000
  H6(H2SiO4)4-2      4.118e-005  1.983e-005   -4.385   -4.703   -0.317
  H2SiO4-2           8.258e-006  3.977e-006   -5.083   -5.400   -0.317
  H4(H2SiO4)4-4      5.069e-006  2.698e-007   -5.295   -6.569   -1.274
```

## A-14. Steel Waste Liners

In order to constrain the number of corrosion scenarios assessed, only four of the effluent solutions from the cement ceiling models were used as inputs to corrosion calculations: (1) fresh cement with minimum ions and rebar, (2) fresh cement with maximum ions and rebar, (3) mature cement with minimum ions and rebar, and (4) mature cement with maximum ions and rebar. For each of these influent solutions, two corrosion scenarios were assessed: carbon steel liners and stainless steel liners. This combination of scenarios yields 8 model input files.

1. Fresh cement (four input files)
   - Minimum ion content, rebar, carbon steel corrosion (file 11)
   - Minimum ion content, rebar, stainless steel corrosion (file 12)
   - Maximum ion content, rebar, carbon steel corrosion (file 13)
   - Maximum ion content, rebar, stainless steel corrosion (file 14)
2. Mature cement (four input files)
   - Minimum ion content, rebar, carbon steel corrosion (file 15)
   - Minimum ion content, rebar, stainless steel corrosion (file 16)
   - Maximum ion content, rebar, carbon steel corrosion (file 17)
   - Maximum ion content, rebar, stainless steel corrosion (file 18)

As with the vault ceiling scenarios, model inputs and results will be presented in order of this file listing. First the input file will be given and then sample results. However, because these models use effluent solutions of previous models as influent solutions, initial results from initial conditions will not be given here (e.g., these results have already been listed previously). Also, note that the input parameters for solution 1 are the same as in the corollary input files previously provided. Results for the final time step will with the last solution be given in the same format as used previously.

**File 11. Fresh Cement, Minimum Ion Content, Cement Rebar, Carbon Steel**

*INPUT FILE*

```
SOLUTION 1
```

```
    temp      15
    pH        7.5
    pe        4
    redox     pe
    units     mmol/kgw
    density   1
    Alkalinity 0
    Cl(-1)    0
    Li        1e-010
    Al        1e-010
    Ca        0.6
    Mg        0.3
    Na        1.3
    K         0
    S(6)      0.3
    N(5)      0
    C(4)      1.4
    Br(-1)    0
    Si        0.01
    -water    1 # kg

GAS_PHASE 1
    -fixed_pressure
    -pressure 1
    -volume 1000
    -temperature 25
    CO2(g)    0.056
    O2(g)     0.18
EQUILIBRIUM_PHASES 1
    Brucite   0 1.39
    Ca(OH)2*(CSH(1.5)) 0 9.5
    Calcite   0 0.001
    CSH(1.0-2.5) 0 15.96
    Gibbsite  0 0.001
    goethite  0 1e-005
    KOH(cement) 0 0.99
    NaOH(cement) 0 0.15
    SiO2(am)  0 0.02
REACTION 1
    Fe        1
    4.75 moles in 60 steps
SAVE solution 1-1
END
USE solution 1
GAS_PHASE 2
    -fixed_pressure
    -pressure 1
    -volume 1000
    -temperature 25
    CO2(g)    0.056
    O2(g)     0.18
EQUILIBRIUM_PHASES 2
    calcite   0 1e-010
    Fe(OH)3   0 1e-010
    goethite  0 1e-010
    portlandite 0 1e-010
    SiO2(am)  0 1e-010
REACTION 3
    Fe        1
    4.05 moles in 60 steps
```

*SAMPLE OUTPUT, FINAL TIME STEP (FILE 11)*

Reaction step 60.

Using solution 1. Solution after simulation 1.
Using pure phase assemblage 2.
Using gas phase 2.
Using reaction 3.

Reaction 3. Irreversible reaction defined in simulation 2.

4.050e+000 moles of the following reaction have been added:

| Reactant | Relative moles |
|---|---|
| Fe | 1.00000 |

| Element | Relative moles |
|---|---|
| Fe | 1.00000 |

----------Gas phase----------

Total pressure: 1.0000 atmospheres
Gas volume: 1.30e+002 liters

| Component | log P | P | Moles in gas Initial | Final | Delta |
|---|---|---|---|---|---|
| CO2(g) | -0.67 | 2.159e-001 | 2.289e+000 | 1.190e+000 | -1.099e+000 |
| O2(g) | -0.11 | 7.841e-001 | 7.357e+000 | 4.320e+000 | -3.037e+000 |

----------Phase assemblage----------

| Phase | SI | log IAP | log KT | Moles in assemblage Initial | Final | Delta |
|---|---|---|---|---|---|---|
| Calcite | -0.00 | 1.98 | 1.98 | 1.000e-010 | 2.825e-005 | 2.825e-005 |
| Fe(OH)3 | -5.26 | 0.89 | 6.15 | 1.000e-010 | 0 | -1.000e-010 |
| Goethite | -0.00 | 0.91 | 0.91 | 1.000e-010 | 4.050e+000 | 4.050e+000 |
| Portlandite | -12.94 | 10.40 | 23.33 | 1.000e-010 | 0 | -1.000e-010 |
| SiO2(am) | 0.00 | -2.87 | -2.87 | 1.000e-010 | 3.615e-002 | 3.615e-002 |

----------Solution composition----------

| Elements | Molality | Moles |
|---|---|---|
| Al | 1.039e-003 | 1.000e-003 |
| C | 1.160e+000 | 1.116e+000 |
| Ca | 1.823e-005 | 1.754e-005 |
| Fe | 8.439e-012 | 8.121e-012 |
| K | 1.029e+000 | 9.900e-001 |
| Li | 1.039e-013 | 1.000e-013 |
| Mg | 3.798e-011 | 3.655e-011 |
| Na | 1.572e-001 | 1.513e-001 |
| S | 3.118e-004 | 3.000e-004 |
| Si | 1.436e-003 | 1.381e-003 |

----------Description of solution----------

```
                              pH  =   8.289      Charge balance
                              pe  =  13.220      Adjusted to redox equilibrium
                   Activity of water  =   0.961
                      Ionic strength  =  1.147e+000
                   Mass of water (kg)  =  9.623e-001
                Total alkalinity (eq/kg)  =  1.187e+000
                    Total CO2 (mol/kg)  =  1.160e+000
                   Temperature (deg C)  =  15.000
                Electrical balance (eq)  =  1.199e-003
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   0.06
                          Iterations  =  28
                            Total H  = 1.079395e+002
                            Total O  = 5.677954e+001

----------------------------Distribution of species----------------------------

                                        Log      Log        Log
  Species              Molality    Activity  Molality  Activity     Gamma

  OH-                1.296e-006  8.228e-007    -5.888    -6.085    -0.197
  H+                 6.246e-009  5.140e-009    -8.204    -8.289    -0.085
  H2O                5.553e+001  9.613e-001     1.744    -0.017     0.000
Al           1.039e-003
  Al13O4(OH)24+7       7.699e-005  2.534e-013    -4.114   -12.596    -8.483
  AlO2-              3.748e-005  2.479e-005    -4.426    -4.606    -0.179
  HAlO2              6.208e-007  6.208e-007    -6.207    -6.207     0.000
  NaAlO2             2.361e-007  2.361e-007    -6.627    -6.627     0.000
  Al(OH)2+           6.335e-009  4.190e-009    -8.198    -8.378    -0.179
  AlOH+2             1.183e-010  1.906e-011    -9.927   -10.720    -0.793
  Al+3               2.418e-013  1.815e-014   -12.617   -13.741    -1.125
  AlSO4+             5.833e-016  3.859e-016   -15.234   -15.414    -0.179
  Al2(OH)2+4           1.894e-016  2.351e-019   -15.723   -18.629    -2.906
  Al3(OH)4+5           1.947e-018  9.633e-023   -17.711   -22.016    -4.306
  Al(SO4)2-          9.407e-019  6.223e-019   -18.027   -18.206    -0.179
C(-2)        0.000e+000
  C2H4               0.000e+000  0.000e+000  -271.782  -271.782     0.000
C(-3)        0.000e+000
  C2H6               0.000e+000  0.000e+000  -243.597  -243.597     0.000
C(-4)        0.000e+000
  CH4                0.000e+000  0.000e+000  -151.959  -151.959     0.000
C(2)         0.000e+000
  CO                 0.000e+000  0.000e+000   -50.317   -50.317     0.000
C(4)         1.160e+000
  HCO3-              1.052e+000  6.956e-001     0.022    -0.158    -0.179
  NaHCO3               6.884e-002  6.884e-002    -1.162    -1.162     0.000
  CO3-2              3.021e-002  4.867e-003    -1.520    -2.313    -0.793
  CO2                7.647e-003  1.001e-002    -2.117    -2.000     0.117
  NaCO3-             1.904e-003  1.260e-003    -2.720    -2.900    -0.179
  CaHCO3+              8.723e-006  5.770e-006    -5.059    -5.239    -0.179
  CaCO3              6.322e-006  6.322e-006    -5.199    -5.199     0.000
  MgHCO3+              2.298e-011  1.520e-011   -10.639   -10.818    -0.179
  MgCO3              8.588e-012  8.588e-012   -11.066   -11.066     0.000
  FeCO3+             1.263e-016  8.352e-017   -15.899   -16.078    -0.179
  FeHCO3+              5.704e-022  3.773e-022   -21.244   -21.423    -0.179
  FeCO3              3.523e-022  3.523e-022   -21.453   -21.453     0.000
Ca           1.823e-005
  CaHCO3+              8.723e-006  5.770e-006    -5.059    -5.239    -0.179
  CaCO3              6.322e-006  6.322e-006    -5.199    -5.199     0.000
  Ca+2               3.178e-006  7.102e-007    -5.498    -6.149    -0.651
  CaSO4              1.968e-009  1.968e-009    -8.706    -8.706     0.000
  CaOH+              2.836e-011  1.876e-011   -10.547   -10.727    -0.179
Fe(2)        9.275e-022
```

| | | | | | |
|---|---|---|---|---|---|
| FeHCO3+ | 5.704e-022 | 3.773e-022 | -21.244 | -21.423 | -0.179 |
| FeCO3 | 3.523e-022 | 3.523e-022 | -21.453 | -21.453 | 0.000 |
| Fe+2 | 4.626e-024 | 1.034e-024 | -23.335 | -23.986 | -0.651 |
| FeOH+ | 9.241e-026 | 6.113e-026 | -25.034 | -25.214 | -0.179 |
| FeSO4 | 3.404e-027 | 3.404e-027 | -26.468 | -26.468 | 0.000 |
| Fe(OH)2 | 9.081e-029 | 9.081e-029 | -28.042 | -28.042 | 0.000 |
| Fe(OH)3- | 1.022e-030 | 6.761e-031 | -29.991 | -30.170 | -0.179 |
| Fe(OH)4-2 | 9.034e-037 | 1.264e-037 | -36.044 | -36.898 | -0.854 |
| Fe(3) | 8.439e-012 | | | | |
| Fe(OH)3 | 7.754e-012 | 7.754e-012 | -11.110 | -11.110 | 0.000 |
| Fe(OH)4- | 5.507e-013 | 3.643e-013 | -12.259 | -12.439 | -0.179 |
| Fe(OH)2+ | 1.340e-013 | 8.865e-014 | -12.873 | -13.052 | -0.179 |
| FeCO3+ | 1.263e-016 | 8.352e-017 | -15.899 | -16.078 | -0.179 |
| FeOH+2 | 8.885e-018 | 1.432e-018 | -17.051 | -17.844 | -0.793 |
| Fe+3 | 1.579e-023 | 1.186e-024 | -22.802 | -23.926 | -1.125 |
| FeSO4+ | 2.466e-027 | 1.631e-027 | -26.608 | -26.788 | -0.179 |
| Fe(SO4)2- | 1.265e-030 | 8.371e-031 | -29.898 | -30.077 | -0.179 |
| Fe2(OH)2+4 | 4.442e-032 | 5.516e-035 | -31.352 | -34.258 | -2.906 |
| Fe3(OH)4+5 | 0.000e+000 | 0.000e+000 | -40.685 | -44.991 | -4.306 |
| H(0) | 0.000e+000 | | | | |
| H2 | 0.000e+000 | 0.000e+000 | -46.444 | -46.327 | 0.117 |
| K | 1.029e+000 | | | | |
| K+ | 1.029e+000 | 6.229e-001 | 0.012 | -0.206 | -0.218 |
| KSO4- | 1.515e-004 | 1.002e-004 | -3.820 | -3.999 | -0.179 |
| KOH | 4.039e-007 | 4.039e-007 | -6.394 | -6.394 | 0.000 |
| KHSO4 | 3.129e-013 | 3.129e-013 | -12.505 | -12.505 | 0.000 |
| Li | 1.039e-013 | | | | |
| Li+ | 1.039e-013 | 7.726e-014 | -12.983 | -13.112 | -0.129 |
| LiSO4- | 1.429e-017 | 9.452e-018 | -16.845 | -17.024 | -0.179 |
| LiOH | 3.310e-019 | 3.310e-019 | -18.480 | -18.480 | 0.000 |
| Mg | 3.798e-011 | | | | |
| MgHCO3+ | 2.298e-011 | 1.520e-011 | -10.639 | -10.818 | -0.179 |
| MgCO3 | 8.588e-012 | 8.588e-012 | -11.066 | -11.066 | 0.000 |
| Mg+2 | 6.408e-012 | 1.924e-012 | -11.193 | -11.716 | -0.522 |
| MgSO4 | 8.201e-015 | 8.201e-015 | -14.086 | -14.086 | 0.000 |
| Mg4(OH)4+4 | 0.000e+000 | 0.000e+000 | -50.619 | -53.525 | -2.906 |
| Na | 1.572e-001 | | | | |
| Na+ | 8.641e-002 | 5.716e-002 | -1.063 | -1.243 | -0.179 |
| NaHCO3 | 6.884e-002 | 6.884e-002 | -1.162 | -1.162 | 0.000 |
| NaCO3- | 1.904e-003 | 1.260e-003 | -2.720 | -2.900 | -0.179 |
| NaHSiO3 | 6.615e-005 | 6.615e-005 | -4.180 | -4.180 | 0.000 |
| NaSO4- | 1.186e-005 | 7.846e-006 | -4.926 | -5.105 | -0.179 |
| NaAlO2 | 2.361e-007 | 2.361e-007 | -6.627 | -6.627 | 0.000 |
| NaOH | 8.317e-009 | 8.317e-009 | -8.080 | -8.080 | 0.000 |
| O(0) | 1.847e-003 | | | | |
| O2 | 9.233e-004 | 1.208e-003 | -3.035 | -2.918 | 0.117 |
| S(-2) | 0.000e+000 | | | | |
| HS- | 0.000e+000 | 0.000e+000 | -150.488 | -150.685 | -0.197 |
| H2S | 0.000e+000 | 0.000e+000 | -151.824 | -151.824 | 0.000 |
| S-2 | 0.000e+000 | 0.000e+000 | -154.884 | -155.623 | -0.739 |
| S2-2 | 0.000e+000 | 0.000e+000 | -267.382 | -268.236 | -0.854 |
| S3-2 | 0.000e+000 | 0.000e+000 | -380.031 | -380.885 | -0.854 |
| S4-2 | 0.000e+000 | 0.000e+000 | -492.912 | -493.766 | -0.854 |
| S5-2 | 0.000e+000 | 0.000e+000 | -606.019 | -606.873 | -0.854 |
| S(2) | 0.000e+000 | | | | |
| S2O3-2 | 0.000e+000 | 0.000e+000 | -157.907 | -158.761 | -0.854 |
| HS2O3- | 0.000e+000 | 0.000e+000 | -165.857 | -166.036 | -0.179 |
| S(3) | 0.000e+000 | | | | |
| S2O4-2 | 0.000e+000 | 0.000e+000 | -143.722 | -144.462 | -0.739 |
| S(4) | 0.000e+000 | | | | |
| SO3-2 | 0.000e+000 | 0.000e+000 | -50.677 | -51.469 | -0.793 |
| HSO3- | 0.000e+000 | 0.000e+000 | -52.401 | -52.580 | -0.179 |

```
   H2SO3              0.000e+000  0.000e+000   -58.834   -58.834     0.000
   SO2               0.000e+000  0.000e+000   -59.070   -59.070     0.000
   S2O6-2             0.000e+000  0.000e+000   -77.146   -78.000    -0.854
   S3O6-2             0.000e+000  0.000e+000  -192.325  -193.179    -0.854
   S4O6-2             0.000e+000  0.000e+000  -291.238  -292.092    -0.854
   S5O6-2             0.000e+000  0.000e+000  -419.657  -420.511    -0.854
S(5)          0.000e+000
   S2O5-2             0.000e+000  0.000e+000  -109.099  -109.953    -0.854
S(6)          3.118e-004
   KSO4-              1.515e-004  1.002e-004    -3.820    -3.999    -0.179
   SO4-2              1.484e-004  2.078e-005    -3.828    -4.682    -0.854
   NaSO4-             1.186e-005  7.846e-006    -4.926    -5.105    -0.179
   CaSO4              1.968e-009  1.968e-009    -8.706    -8.706     0.000
   HSO4-              1.231e-011  8.143e-012   -10.910   -11.089    -0.179
   KHSO4              3.129e-013  3.129e-013   -12.505   -12.505     0.000
   MgSO4              8.201e-015  8.201e-015   -14.086   -14.086     0.000
   AlSO4+             5.833e-016  3.859e-016   -15.234   -15.414    -0.179
   LiSO4-             1.429e-017  9.452e-018   -16.845   -17.024    -0.179
   Al(SO4)2-          9.407e-019  6.223e-019   -18.027   -18.206    -0.179
   H2SO4              5.231e-023  5.231e-023   -22.281   -22.281     0.000
   FeSO4              3.404e-027  3.404e-027   -26.468   -26.468     0.000
   FeSO4+             2.466e-027  1.631e-027   -26.608   -26.788    -0.179
   Fe(SO4)2-          1.265e-030  8.371e-031   -29.898   -30.077    -0.179
S(7)          0.000e+000
   S2O8-2             0.000e+000  0.000e+000   -50.168   -51.022    -0.854
S(8)          4.356e-033
   HSO5-              4.356e-033  2.881e-033   -32.361   -32.540    -0.179
Si            1.436e-003
   SiO2              1.339e-003  1.339e-003    -2.873    -2.873     0.000
   NaHSiO3            6.615e-005  6.615e-005    -4.180    -4.180     0.000
   HSiO3-             3.055e-005  2.021e-005    -4.515    -4.694    -0.179
   H6(H2SiO4)4-2      1.451e-008  2.031e-009    -7.838    -8.692    -0.854
   H2SiO4-2           3.668e-009  5.134e-010    -8.436    -9.290    -0.854
   H4(H2SiO4)4-4      1.373e-011  3.852e-015   -10.862   -14.414    -3.552
```

## File 12. Fresh Cement, Minimum Ion Content, Cement Rebar, Stainless Steel

*INPUT FILE*

```
SOLUTION 1
    temp      15
    pH        7.5
    pe        4
    redox     pe
    units     mmol/kgw
    density   1
    Alkalinity 0
    Cl(-1)    0
    Li        1e-010
    Al        1e-010
    Ca        0.6
    Mg        0.3
    Na        1.3
    K         0
    S(6)      0.3
    N(5)      0
    C(4)      1.4
    Br(-1)    0
    Si        0.01
    -water    1 # kg

GAS_PHASE 1
```

```
    -fixed_pressure
    -pressure 1
    -volume 1000
    -temperature 25
    CO2(g)    0.056
    O2(g)     0.18
EQUILIBRIUM_PHASES 1
    Brucite   0 1.39
    Ca(OH)2*(CSH(1.5)) 0 9.5
    Calcite   0 0.001
    CSH(1.0-2.5) 0 15.96
    Gibbsite  0 0.001
    goethite  0 1e-005
    KOH(cement) 0 0.99
    NaOH(cement) 0 0.15
    SiO2(am)  0 0.02
REACTION 1
    Fe        1
    4.75 moles in 60 steps
SAVE solution 1-1
END
USE solution 1
GAS_PHASE 2
    -fixed_pressure
    -pressure 1
    -volume 1000
    -temperature 25
    CO2(g)    0.056
    O2(g)     0.18
EQUILIBRIUM_PHASES 2
    calcite   0 1e-010
    Fe(OH)3   0 1e-010
    goethite  0 1e-010
    portlandite 0 1e-010
    SiO2(am)  0 1e-010
REACTION 3
    Fe        1
    0.025 moles in 60 steps
```

## *SAMPLE OUTPUT, FINAL TIME STEP (FILE 12)*

```
Reaction step 60.

Using solution 1.       Solution after simulation 1.
Using pure phase assemblage 2.
Using gas phase 2.   Gas phase after simulation 2.
Using reaction 3.

Reaction 3.       Irreversible reaction defined in simulation 2.

      2.500e-002 moles of the following reaction have been added:

                  Relative
      Reactant          moles

      Fe              1.00000

                  Relative
      Element           moles
      Fe              1.00000

-----------------------------------Gas phase-----------------------------------
```

Total pressure: 0.9509 atmospheres
Gas volume: 9.00e+000 liters

| Component | log P | P | Moles in gas Initial | Final | Delta |
|---|---|---|---|---|---|
| CO2(g) | -12.55 | 2.846e-013 | 1.084e-013 | 1.083e-013 | -2.380e-017 |
| O2(g) | -0.02 | 9.509e-001 | 3.806e-001 | 3.619e-001 | -1.869e-002 |

----------Phase assemblage----------

| Phase | SI log IAP | log KT | Moles in assemblage Initial | Final | Delta |
|---|---|---|---|---|---|
| Calcite | 0.00 1.98 | 1.98 | 1.000e-010 | 1.006e-008 | 9.962e-009 |
| Fe(OH)3 | -5.26 0.89 | 6.15 | 1.000e-010 | 0 | -1.000e-010 |
| Goethite | 0.00 0.91 | 0.91 | 1.000e-010 | 2.500e-002 | 2.500e-002 |
| Portlandite | -1.05 22.28 | 23.33 | 1.000e-010 | 0 | -1.000e-010 |
| SiO2(am) | -4.60 -7.48 | -2.87 | 1.000e-010 | 0 | -1.000e-010 |

----------Solution composition----------

| Elements | Molality | Moles |
|---|---|---|
| Al | 1.002e-003 | 1.000e-003 |
| C | 1.716e-002 | 1.713e-002 |
| Ca | 4.585e-005 | 4.578e-005 |
| Fe | 3.529e-007 | 3.523e-007 |
| K | 9.917e-001 | 9.900e-001 |
| Li | 1.002e-013 | 1.000e-013 |
| Mg | 3.661e-011 | 3.655e-011 |
| Na | 1.516e-001 | 1.513e-001 |
| S | 3.005e-004 | 3.000e-004 |
| Si | 3.760e-002 | 3.753e-002 |

----------Description of solution----------

pH = 14.093 Charge balance
pe = 7.436 Adjusted to redox equilibrium
Activity of water = 0.966
Ionic strength = 9.815e-001
Mass of water (kg) = 9.983e-001
Total alkalinity (eq/kg) = 1.145e+000
Total CO2 (mol/kg) = 1.716e-002
Temperature (deg C) = 15.000
Electrical balance (eq) = 1.199e-003
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 0.06
Iterations = 5
Total H = 1.119645e+002
Total O = 5.666642e+001

----------Distribution of species----------

| Species | Molality | Log Activity | Log Molality | Log Activity | Gamma |
|---|---|---|---|---|---|
| OH- | 8.244e-001 | 5.259e-001 | -0.084 | -0.279 | -0.195 |
| H+ | 9.908e-015 | 8.078e-015 | -14.004 | -14.093 | -0.089 |
| H2O | 5.553e+001 | 9.656e-001 | 1.744 | -0.015 | 0.000 |

| | | | | | |
|---|---|---|---|---|---|
| Al | 1.002e-003 | | | | |
| AlO2- | 9.916e-004 | 6.571e-004 | -3.004 | -3.182 | -0.179 |
| NaAlO2 | 1.013e-005 | 1.013e-005 | -4.994 | -4.994 | 0.000 |
| HAlO2 | 2.586e-011 | 2.586e-011 | -10.587 | -10.587 | 0.000 |
| Al(OH)2+ | 4.140e-019 | 2.743e-019 | -18.383 | -18.562 | -0.179 |
| AlOH+2 | 1.160e-026 | 1.952e-027 | -25.936 | -26.709 | -0.774 |
| Al+3 | 3.736e-035 | 2.908e-036 | -34.428 | -35.536 | -1.109 |
| AlSO4+ | 1.011e-037 | 6.702e-038 | -36.995 | -37.174 | -0.179 |
| Al(SO4)2- | 1.768e-040 | 1.172e-040 | -39.753 | -39.931 | -0.179 |
| Al2(OH)2+4 | 0.000e+000 | 0.000e+000 | -47.775 | -50.608 | -2.833 |
| Al3(OH)4+5 | 0.000e+000 | 0.000e+000 | -59.978 | -64.179 | -4.202 |
| Al13O4(OH)24+7 | 0.000e+000 | 0.000e+000 | -101.890 | -110.162 | -8.272 |
| C(-2) | 0.000e+000 | | | | |
| C2H4 | 0.000e+000 | 0.000e+000 | -295.790 | -295.790 | 0.000 |
| C(-3) | 0.000e+000 | | | | |
| C2H6 | 0.000e+000 | 0.000e+000 | -267.644 | -267.644 | 0.000 |
| C(-4) | 0.000e+000 | | | | |
| CH4 | 0.000e+000 | 0.000e+000 | -164.002 | -164.002 | 0.000 |
| C(2) | 0.000e+000 | | | | |
| CO | 0.000e+000 | 0.000e+000 | -62.239 | -62.239 | 0.000 |
| C(4) | 1.716e-002 | | | | |
| CO3-2 | 1.550e-002 | 2.609e-003 | -1.810 | -2.583 | -0.774 |
| NaCO3- | 1.649e-003 | 1.093e-003 | -2.783 | -2.962 | -0.179 |
| CaCO3 | 6.322e-006 | 6.322e-006 | -5.199 | -5.199 | 0.000 |
| HCO3- | 8.844e-007 | 5.861e-007 | -6.053 | -6.232 | -0.179 |
| NaHCO3 | 9.386e-008 | 9.386e-008 | -7.028 | -7.028 | 0.000 |
| MgCO3 | 1.540e-011 | 1.540e-011 | -10.812 | -10.812 | 0.000 |
| CaHCO3+ | 1.368e-011 | 9.069e-012 | -10.864 | -11.042 | -0.179 |
| CO2 | 1.047e-014 | 1.319e-014 | -13.980 | -13.880 | 0.100 |
| MgHCO3+ | 6.465e-017 | 4.284e-017 | -16.189 | -16.368 | -0.179 |
| FeCO3 | 4.416e-034 | 4.416e-034 | -33.355 | -33.355 | 0.000 |
| FeCO3+ | 2.599e-034 | 1.722e-034 | -33.585 | -33.764 | -0.179 |
| FeHCO3+ | 1.122e-039 | 7.432e-040 | -38.950 | -39.129 | -0.179 |
| Ca | 4.585e-005 | | | | |
| CaOH+ | 3.375e-005 | 2.237e-005 | -4.472 | -4.650 | -0.179 |
| CaCO3 | 6.322e-006 | 6.322e-006 | -5.199 | -5.199 | 0.000 |
| Ca+2 | 5.778e-006 | 1.325e-006 | -5.238 | -5.878 | -0.640 |
| CaSO4 | 3.979e-009 | 3.979e-009 | -8.400 | -8.400 | 0.000 |
| CaHCO3+ | 1.368e-011 | 9.069e-012 | -10.864 | -11.042 | -0.179 |
| Fe(2) | 9.573e-025 | | | | |
| Fe(OH)3- | 6.228e-025 | 4.127e-025 | -24.206 | -24.384 | -0.179 |
| Fe(OH)4-2 | 3.345e-025 | 4.933e-026 | -24.476 | -25.307 | -0.831 |
| Fe(OH)2 | 8.673e-029 | 8.673e-029 | -28.062 | -28.062 | 0.000 |
| FeOH+ | 1.378e-031 | 9.134e-032 | -30.861 | -31.039 | -0.179 |
| FeCO3 | 4.416e-034 | 4.416e-034 | -33.355 | -33.355 | 0.000 |
| Fe+2 | 1.054e-035 | 2.416e-036 | -34.977 | -35.617 | -0.640 |
| FeSO4 | 8.625e-039 | 8.625e-039 | -38.064 | -38.064 | 0.000 |
| FeHCO3+ | 1.122e-039 | 7.432e-040 | -38.950 | -39.129 | -0.179 |
| Fe(3) | 3.529e-007 | | | | |
| Fe(OH)4- | 3.529e-007 | 2.339e-007 | -6.452 | -6.631 | -0.179 |
| Fe(OH)3 | 7.790e-012 | 7.790e-012 | -11.108 | -11.108 | 0.000 |
| Fe(OH)2+ | 2.102e-019 | 1.393e-019 | -18.677 | -18.856 | -0.179 |
| FeOH+2 | 2.091e-029 | 3.520e-030 | -28.680 | -29.453 | -0.774 |
| FeCO3+ | 2.599e-034 | 1.722e-034 | -33.585 | -33.764 | -0.179 |
| Fe+3 | 0.000e+000 | 0.000e+000 | -40.232 | -41.341 | -1.109 |
| FeSO4+ | 0.000e+000 | 0.000e+000 | -43.989 | -44.167 | -0.179 |
| Fe(SO4)2- | 0.000e+000 | 0.000e+000 | -47.243 | -47.422 | -0.179 |
| Fe2(OH)2+4 | 0.000e+000 | 0.000e+000 | -54.644 | -57.477 | -2.833 |
| Fe3(OH)4+5 | 0.000e+000 | 0.000e+000 | -69.811 | -74.013 | -4.202 |
| H(0) | 0.000e+000 | | | | |
| H2 | 0.000e+000 | 0.000e+000 | -46.467 | -46.367 | 0.100 |
| K | 9.917e-001 | | | | |

| | | | | | |
|---|---|---|---|---|---|
| K+ | 7.914e-001 | 4.830e-001 | -0.102 | -0.316 | -0.214 |
| KOH | 2.002e-001 | 2.002e-001 | -0.699 | -0.699 | 0.000 |
| KSO4- | 1.271e-004 | 8.421e-005 | -3.896 | -4.075 | -0.179 |
| KHSO4 | 4.133e-019 | 4.133e-019 | -18.384 | -18.384 | 0.000 |
| Li | 1.002e-013 | | | | |
| LiOH | 6.707e-014 | 6.707e-014 | -13.173 | -13.173 | 0.000 |
| Li+ | 3.310e-014 | 2.449e-014 | -13.480 | -13.611 | -0.131 |
| LiSO4- | 4.901e-018 | 3.248e-018 | -17.310 | -17.488 | -0.179 |
| Mg | 3.661e-011 | | | | |
| Mg+2 | 2.118e-011 | 6.437e-012 | -10.674 | -11.191 | -0.517 |
| MgCO3 | 1.540e-011 | 1.540e-011 | -10.812 | -10.812 | 0.000 |
| MgSO4 | 2.974e-014 | 2.974e-014 | -13.527 | -13.527 | 0.000 |
| MgHCO3+ | 6.465e-017 | 4.284e-017 | -16.189 | -16.368 | -0.179 |
| Mg4(OH)4+4 | 4.245e-026 | 6.234e-029 | -25.372 | -28.205 | -2.833 |
| Na | 1.516e-001 | | | | |
| Na+ | 1.396e-001 | 9.250e-002 | -0.855 | -1.034 | -0.179 |
| NaOH | 8.602e-003 | 8.602e-003 | -2.065 | -2.065 | 0.000 |
| NaHSiO3 | 1.704e-003 | 1.704e-003 | -2.769 | -2.769 | 0.000 |
| NaCO3- | 1.649e-003 | 1.093e-003 | -2.783 | -2.962 | -0.179 |
| NaSO4- | 2.077e-005 | 1.376e-005 | -4.683 | -4.861 | -0.179 |
| NaAlO2 | 1.013e-005 | 1.013e-005 | -4.994 | -4.994 | 0.000 |
| NaHCO3 | 9.386e-008 | 9.386e-008 | -7.028 | -7.028 | 0.000 |
| O(0) | 2.326e-003 | | | | |
| O2 | 1.163e-003 | 1.465e-003 | -2.934 | -2.834 | 0.100 |
| S(-2) | 0.000e+000 | | | | |
| S-2 | 0.000e+000 | 0.000e+000 | -155.032 | -155.756 | -0.724 |
| HS- | 0.000e+000 | 0.000e+000 | -156.426 | -156.622 | -0.195 |
| H2S | 0.000e+000 | 0.000e+000 | -163.564 | -163.564 | 0.000 |
| S2-2 | 0.000e+000 | 0.000e+000 | -279.237 | -280.068 | -0.831 |
| S3-2 | 0.000e+000 | 0.000e+000 | -403.587 | -404.418 | -0.831 |
| S4-2 | 0.000e+000 | 0.000e+000 | -528.167 | -528.998 | -0.831 |
| S5-2 | 0.000e+000 | 0.000e+000 | -652.974 | -653.805 | -0.831 |
| S(2) | 0.000e+000 | | | | |
| S2O3-2 | 0.000e+000 | 0.000e+000 | -169.637 | -170.468 | -0.831 |
| HS2O3- | 0.000e+000 | 0.000e+000 | -183.368 | -183.547 | -0.179 |
| S(3) | 0.000e+000 | | | | |
| S2O4-2 | 0.000e+000 | 0.000e+000 | -155.403 | -156.127 | -0.724 |
| S(4) | 0.000e+000 | | | | |
| SO3-2 | 0.000e+000 | 0.000e+000 | -50.703 | -51.476 | -0.774 |
| HSO3- | 0.000e+000 | 0.000e+000 | -58.212 | -58.391 | -0.179 |
| H2SO3 | 0.000e+000 | 0.000e+000 | -70.449 | -70.449 | 0.000 |
| SO2 | 0.000e+000 | 0.000e+000 | -70.687 | -70.687 | 0.000 |
| S2O6-2 | 0.000e+000 | 0.000e+000 | -88.750 | -89.582 | -0.831 |
| S3O6-2 | 0.000e+000 | 0.000e+000 | -215.629 | -216.460 | -0.831 |
| S4O6-2 | 0.000e+000 | 0.000e+000 | -326.242 | -327.073 | -0.831 |
| S5O6-2 | 0.000e+000 | 0.000e+000 | -466.361 | -467.192 | -0.831 |
| S(5) | 0.000e+000 | | | | |
| S2O5-2 | 0.000e+000 | 0.000e+000 | -120.745 | -121.576 | -0.831 |
| S(6) | 3.005e-004 | | | | |
| SO4-2 | 1.527e-004 | 2.252e-005 | -3.816 | -4.647 | -0.831 |
| KSO4- | 1.271e-004 | 8.421e-005 | -3.896 | -4.075 | -0.179 |
| NaSO4- | 2.077e-005 | 1.376e-005 | -4.683 | -4.861 | -0.179 |
| CaSO4 | 3.979e-009 | 3.979e-009 | -8.400 | -8.400 | 0.000 |
| MgSO4 | 2.974e-014 | 2.974e-014 | -13.527 | -13.527 | 0.000 |
| HSO4- | 2.093e-017 | 1.387e-017 | -16.679 | -16.858 | -0.179 |
| LiSO4- | 4.901e-018 | 3.248e-018 | -17.310 | -17.488 | -0.179 |
| KHSO4 | 4.133e-019 | 4.133e-019 | -18.384 | -18.384 | 0.000 |
| H2SO4 | 1.401e-034 | 1.401e-034 | -33.854 | -33.854 | 0.000 |
| AlSO4+ | 1.011e-037 | 6.702e-038 | -36.995 | -37.174 | -0.179 |
| FeSO4 | 8.625e-039 | 8.625e-039 | -38.064 | -38.064 | 0.000 |
| Al(SO4)2- | 1.768e-040 | 1.172e-040 | -39.753 | -39.931 | -0.179 |
| FeSO4+ | 0.000e+000 | 0.000e+000 | -43.989 | -44.167 | -0.179 |

```
  Fe(SO4)2-          0.000e+000  0.000e+000   -47.243   -47.422    -0.179
S(7)          0.000e+000
  S2O8-2             0.000e+000  0.000e+000   -61.689   -62.520    -0.831
S(8)          8.157e-039
  HSO5-              8.157e-039  5.405e-039   -38.088   -38.267    -0.179
Si            3.760e-002
  H2SiO4-2           3.541e-002  5.223e-003    -1.451    -2.282    -0.831
  NaHSiO3            1.704e-003  1.704e-003    -2.769    -2.769     0.000
  HSiO3-             4.854e-004  3.217e-004    -3.314    -3.493    -0.179
  H4(H2SiO4)4-4      6.953e-007  2.517e-010    -6.158    -9.599    -3.441
  SiO2               3.334e-008  3.334e-008    -7.477    -7.477     0.000
  H6(H2SiO4)4-2      2.222e-015  3.277e-016   -14.653   -15.484    -0.831
```

## File 13. Fresh Cement, Maximum Ion Content, Cement Rebar, Carbon Steel

*INPUT FILE*

```
SOLUTION 1
   temp      15
   pH        7.5
   pe        4
   redox     pe
   units     mmol/kgw
   density   1
   Alkalinity 0
   Cl(-1)    7.5
   Li        1e-010
   Al        1e-010
   Ca        3.1
   Mg        5
   Na        18
   K         1.9
   S(6)      7.3
   N(5)      7.9
   C(4)      21.8
   Br(-1)    0
   Si        0.01
   -water    1 # kg

GAS_PHASE 1
   -fixed_pressure
   -pressure 1
   -volume 1000
   -temperature 25
   CO2(g)    0.056
   O2(g)     0.18
EQUILIBRIUM_PHASES 1
   Brucite   0 1.39
   Ca(OH)2*(CSH(1.5)) 0 9.5
   Calcite   0 0.001
   CSH(1.0-2.5) 0 15.96
   Gibbsite  0 0.001
   goethite  0 1e-005
   KOH(cement) 0 0.99
   NaOH(cement) 0 0.15
   SiO2(am)  0 0.02
   Siderite  0 1e-010
REACTION 1
   Fe        1
   4.75 moles in 60 steps
SAVE solution 1-1
END
```

```
USE solution 1
GAS_PHASE 2
   -fixed_pressure
   -pressure 1
   -volume 1000
   -temperature 25
   CO2(g)    0.056
   O2(g)     0.18
EQUILIBRIUM_PHASES 2
   Albite    0 1e-010
   Beidellite-K 0 1e-010
   calcite   0 1e-010
   Fe(OH)3   0 1e-010
   goethite  0 1e-010
   K2CO3:1.5H2O 0 1e-010
   Na2CO3    0 1e-010
   Na2CO3:7H2O 0 1e-010
   Nahcolite 0 1e-010
   portlandite 0 1e-010
   SiO2(am)  0 1e-010
   Illite    0 1e-010
REACTION 3
   Fe        1
   4.05 moles in 60 steps
```

*SAMPLE OUTPUT, FINAL TIME STEP (FILE 13)*

```
Reaction step 60.

Using solution 1.       Solution after simulation 1.
Using pure phase assemblage 2.
Using gas phase 2.
Using reaction 3.

Reaction 3.       Irreversible reaction defined in simulation 2.

      4.050e+000 moles of the following reaction have been added:

                  Relative
      Reactant       moles

      Fe            1.00000

                  Relative
      Element        moles
      Fe            1.00000

-----------------------------------Gas phase-----------------------------------


Total pressure:   1.0000   atmospheres
   Gas volume:  1.30e+002 liters

                                        Moles in gas
                                  ----------------------------------
Component             log P          P     Initial      Final       Delta

CO2(g)                -0.67  2.155e-001  2.289e+000  1.187e+000 -1.102e+000
O2(g)                 -0.11  7.845e-001  7.357e+000  4.320e+000 -3.037e+000

-----------------------------Phase assemblage-----------------------------
```

| Phase | SI | log IAP | log KT | Moles in assemblage: Initial | Final | Delta |
|---|---|---|---|---|---|---|
| Albite | -0.00 | 2.94 | 2.94 | 1.000e-010 | 1.000e-003 | 1.000e-003 |
| Beidellite-K | -3.50 | 2.55 | 6.05 | 1.000e-010 | 0 | -1.000e-010 |
| Calcite | -0.00 | 1.98 | 1.98 | 1.000e-010 | 2.826e-005 | 2.826e-005 |
| Fe(OH)3 | -5.26 | 0.89 | 6.15 | 1.000e-010 | 0 | -1.000e-010 |
| Goethite | -0.00 | 0.91 | 0.91 | 1.000e-010 | 4.050e+000 | 4.050e+000 |
| Illite | -3.54 | 6.35 | 9.89 | 1.000e-010 | 0 | -1.000e-010 |
| K2CO3:1.5H2O | -5.69 | 7.69 | 13.38 | 1.000e-010 | 0 | -1.000e-010 |
| Na2CO3 | -5.68 | 5.73 | 11.41 | 1.000e-010 | 0 | -1.000e-010 |
| Na2CO3:7H2O | -4.18 | 5.61 | 9.79 | 1.000e-010 | 0 | -1.000e-010 |
| Nahcolite | -1.12 | -1.36 | -0.24 | 1.000e-010 | 0 | -1.000e-010 |
| Portlandite | -12.94 | 10.40 | 23.33 | 1.000e-010 | 0 | -1.000e-010 |
| SiO2(am) | 0.00 | -2.87 | -2.87 | 1.000e-010 | 3.377e-002 | 3.377e-002 |

----------Solution composition----------

| Elements | Molality | Moles |
|---|---|---|
| Al | 9.276e-012 | 8.930e-012 |
| C | 1.163e+000 | 1.120e+000 |
| Ca | 1.834e-005 | 1.765e-005 |
| Cl | 7.791e-003 | 7.500e-003 |
| Fe | 8.433e-012 | 8.118e-012 |
| K | 1.030e+000 | 9.919e-001 |
| Li | 1.039e-013 | 1.000e-013 |
| Mg | 6.467e-011 | 6.226e-011 |
| N | 8.207e-003 | 7.900e-003 |
| Na | 1.735e-001 | 1.670e-001 |
| S | 7.583e-003 | 7.300e-003 |
| Si | 1.442e-003 | 1.388e-003 |

----------Description of solution----------

pH = 8.288 Charge balance
pe = 13.221 Adjusted to redox equilibrium
Activity of water = 0.961
Ionic strength = 1.163e+000
Mass of water (kg) = 9.627e-001
Total alkalinity (eq/kg) = 1.188e+000
Total CO2 (mol/kg) = 1.163e+000
Temperature (deg C) = 15.000
Electrical balance (eq) = -1.448e-002
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.67
Iterations = 34
Total H = 1.079843e+002
Total O = 5.686047e+001

----------Distribution of species----------

| Species | Molality | Log Activity | Log Molality | Log Activity | Gamma |
|---|---|---|---|---|---|
| OH- | 1.293e-006 | 8.212e-007 | -5.888 | -6.086 | -0.197 |
| H+ | 6.249e-009 | 5.147e-009 | -8.204 | -8.288 | -0.084 |
| H2O | 5.553e+001 | 9.607e-001 | 1.744 | -0.017 | 0.000 |
| Al | 9.276e-012 | | | | |
| AlO2- | 9.062e-012 | 5.994e-012 | -11.043 | -11.222 | -0.179 |
| HAlO2 | 1.503e-013 | 1.503e-013 | -12.823 | -12.823 | 0.000 |
| NaAlO2 | 6.297e-014 | 6.297e-014 | -13.201 | -13.201 | 0.000 |
| Al(OH)2+ | 1.536e-015 | 1.016e-015 | -14.814 | -14.993 | -0.179 |

| | | | | | |
|---|---|---|---|---|---|
| AlOH+2 | 2.885e-017 | 4.631e-018 | -16.540 | -17.334 | -0.794 |
| Al+3 | 5.903e-020 | 4.418e-021 | -19.229 | -20.355 | -1.126 |
| AlSO4+ | 3.437e-021 | 2.274e-021 | -20.464 | -20.643 | -0.179 |
| Al(SO4)2- | 1.342e-022 | 8.876e-023 | -21.872 | -22.052 | -0.179 |
| Al2(OH)2+4 | 1.134e-029 | 1.388e-032 | -28.945 | -31.858 | -2.912 |
| Al3(OH)4+5 | 2.847e-038 | 0.000e+000 | -37.546 | -41.861 | -4.315 |
| Al13O4(OH)24+7 | 0.000e+000 | 0.000e+000 | -90.099 | -98.600 | -8.501 |
| C(-2) | 0.000e+000 | | | | |
| C2H4 | 0.000e+000 | 0.000e+000 | -271.785 | -271.785 | 0.000 |
| C(-3) | 0.000e+000 | | | | |
| C2H6 | 0.000e+000 | 0.000e+000 | -243.600 | -243.600 | 0.000 |
| C(-4) | 0.000e+000 | | | | |
| CH4 | 0.000e+000 | 0.000e+000 | -151.961 | -151.961 | 0.000 |
| C(2) | 0.000e+000 | | | | |
| CO | 0.000e+000 | 0.000e+000 | -50.318 | -50.318 | 0.000 |
| C(4) | 1.163e+000 | | | | |
| HCO3- | 1.048e+000 | 6.929e-001 | 0.020 | -0.159 | -0.179 |
| NaHCO3 | 7.564e-002 | 7.564e-002 | -1.121 | -1.121 | 0.000 |
| CO3-2 | 3.016e-002 | 4.841e-003 | -1.521 | -2.315 | -0.794 |
| CO2 | 7.604e-003 | 9.987e-003 | -2.119 | -2.001 | 0.118 |
| NaCO3- | 2.089e-003 | 1.382e-003 | -2.680 | -2.860 | -0.179 |
| CaHCO3+ | 8.736e-006 | 5.779e-006 | -5.059 | -5.238 | -0.179 |
| CaCO3 | 6.322e-006 | 6.322e-006 | -5.199 | -5.199 | 0.000 |
| MgHCO3+ | 3.890e-011 | 2.573e-011 | -10.410 | -10.590 | -0.179 |
| MgCO3 | 1.452e-011 | 1.452e-011 | -10.838 | -10.838 | 0.000 |
| FeCO3+ | 1.263e-016 | 8.353e-017 | -15.899 | -16.078 | -0.179 |
| FeHCO3+ | 5.703e-022 | 3.772e-022 | -21.244 | -21.423 | -0.179 |
| FeCO3 | 3.517e-022 | 3.517e-022 | -21.454 | -21.454 | 0.000 |
| Ca | 1.834e-005 | | | | |
| CaHCO3+ | 8.736e-006 | 5.779e-006 | -5.059 | -5.238 | -0.179 |
| CaCO3 | 6.322e-006 | 6.322e-006 | -5.199 | -5.199 | 0.000 |
| Ca+2 | 3.202e-006 | 7.139e-007 | -5.495 | -6.146 | -0.652 |
| CaSO4 | 4.789e-008 | 4.789e-008 | -7.320 | -7.320 | 0.000 |
| CaNO3+ | 2.686e-008 | 1.777e-008 | -7.571 | -7.750 | -0.179 |
| CaCl+ | 1.034e-009 | 6.840e-010 | -8.985 | -9.165 | -0.179 |
| CaOH+ | 2.845e-011 | 1.882e-011 | -10.546 | -10.725 | -0.179 |
| CaCl2 | 4.159e-012 | 4.159e-012 | -11.381 | -11.381 | 0.000 |
| Cl(-1) | 7.791e-003 | | | | |
| Cl- | 7.665e-003 | 4.638e-003 | -2.116 | -2.334 | -0.218 |
| KCl | 7.863e-005 | 7.863e-005 | -4.104 | -4.104 | 0.000 |
| NaCl | 4.764e-005 | 4.764e-005 | -4.322 | -4.322 | 0.000 |
| CaCl+ | 1.034e-009 | 6.840e-010 | -8.985 | -9.165 | -0.179 |
| HCl | 5.262e-012 | 5.262e-012 | -11.279 | -11.279 | 0.000 |
| CaCl2 | 4.159e-012 | 4.159e-012 | -11.381 | -11.381 | 0.000 |
| MgCl+ | 1.817e-014 | 1.202e-014 | -13.741 | -13.920 | -0.179 |
| LiCl | 1.091e-017 | 1.091e-017 | -16.962 | -16.962 | 0.000 |
| FeCl2+ | 5.230e-027 | 3.459e-027 | -26.282 | -26.461 | -0.179 |
| FeCl+ | 5.093e-027 | 3.369e-027 | -26.293 | -26.473 | -0.179 |
| FeCl+2 | 3.434e-027 | 5.513e-028 | -26.464 | -27.259 | -0.794 |
| FeCl2 | 7.970e-032 | 7.970e-032 | -31.099 | -31.099 | 0.000 |
| FeCl4- | 1.353e-034 | 8.947e-035 | -33.869 | -34.048 | -0.179 |
| FeCl4-2 | 3.509e-035 | 4.888e-036 | -34.455 | -35.311 | -0.856 |
| Cl(1) | 8.409e-020 | | | | |
| ClO- | 7.466e-020 | 4.939e-020 | -19.127 | -19.306 | -0.179 |
| HClO | 9.428e-021 | 9.428e-021 | -20.026 | -20.026 | 0.000 |
| Cl(3) | 1.319e-029 | | | | |
| ClO2- | 1.319e-029 | 8.723e-030 | -28.880 | -29.059 | -0.179 |
| HClO2 | 6.638e-035 | 6.638e-035 | -34.178 | -34.178 | 0.000 |
| Cl(5) | 5.195e-025 | | | | |
| ClO3- | 5.195e-025 | 3.298e-025 | -24.284 | -24.482 | -0.197 |
| Cl(7) | 8.238e-025 | | | | |
| ClO4- | 8.238e-025 | 5.231e-025 | -24.084 | -24.281 | -0.197 |

| | | | | | |
|---|---|---|---|---|---|
| Fe(2) | 9.269e-022 | | | | |
| FeHCO3+ | 5.703e-022 | 3.772e-022 | -21.244 | -21.423 | -0.179 |
| FeCO3 | 3.517e-022 | 3.517e-022 | -21.454 | -21.454 | 0.000 |
| Fe+2 | 4.652e-024 | 1.037e-024 | -23.332 | -23.984 | -0.652 |
| FeOH+ | 9.256e-026 | 6.123e-026 | -25.034 | -25.213 | -0.179 |
| FeSO4 | 8.268e-026 | 8.268e-026 | -25.083 | -25.083 | 0.000 |
| FeCl+ | 5.093e-027 | 3.369e-027 | -26.293 | -26.473 | -0.179 |
| Fe(OH)2 | 9.077e-029 | 9.077e-029 | -28.042 | -28.042 | 0.000 |
| Fe(OH)3- | 1.020e-030 | 6.744e-031 | -29.992 | -30.171 | -0.179 |
| FeCl2 | 7.970e-032 | 7.970e-032 | -31.099 | -31.099 | 0.000 |
| FeCl4-2 | 3.509e-035 | 4.888e-036 | -34.455 | -35.311 | -0.856 |
| Fe(OH)4-2 | 9.035e-037 | 1.259e-037 | -36.044 | -36.900 | -0.856 |
| Fe(3) | 8.433e-012 | | | | |
| Fe(OH)3 | 7.750e-012 | 7.750e-012 | -11.111 | -11.111 | 0.000 |
| Fe(OH)4- | 5.493e-013 | 3.633e-013 | -12.260 | -12.440 | -0.179 |
| Fe(OH)2+ | 1.342e-013 | 8.877e-014 | -12.872 | -13.052 | -0.179 |
| FeCO3+ | 1.263e-016 | 8.353e-017 | -15.899 | -16.078 | -0.179 |
| FeOH+2 | 8.949e-018 | 1.436e-018 | -17.048 | -17.843 | -0.794 |
| Fe+3 | 1.593e-023 | 1.192e-024 | -22.798 | -23.924 | -1.126 |
| FeNO3+2 | 3.688e-025 | 5.920e-026 | -24.433 | -25.228 | -0.794 |
| FeSO4+ | 6.001e-026 | 3.970e-026 | -25.222 | -25.401 | -0.179 |
| FeCl2+ | 5.230e-027 | 3.459e-027 | -26.282 | -26.461 | -0.179 |
| FeCl+2 | 3.434e-027 | 5.513e-028 | -26.464 | -27.259 | -0.794 |
| Fe(SO4)2- | 7.455e-028 | 4.931e-028 | -27.128 | -27.307 | -0.179 |
| Fe2(OH)2+4 | 4.540e-032 | 5.554e-035 | -31.343 | -34.255 | -2.912 |
| FeCl4- | 1.353e-034 | 8.947e-035 | -33.869 | -34.048 | -0.179 |
| FeNO2+2 | 2.299e-037 | 3.690e-038 | -36.639 | -37.433 | -0.794 |
| Fe3(OH)4+5 | 0.000e+000 | 0.000e+000 | -40.672 | -44.987 | -4.315 |
| H(0) | 0.000e+000 | | | | |
| H2 | 0.000e+000 | 0.000e+000 | -46.446 | -46.328 | 0.118 |
| K | 1.030e+000 | | | | |
| K+ | 1.027e+000 | 6.213e-001 | 0.011 | -0.207 | -0.218 |
| KSO4- | 3.657e-003 | 2.419e-003 | -2.437 | -2.616 | -0.179 |
| KCl | 7.863e-005 | 7.863e-005 | -4.104 | -4.104 | 0.000 |
| KOH | 4.020e-007 | 4.020e-007 | -6.396 | -6.396 | 0.000 |
| KHSO4 | 7.564e-012 | 7.564e-012 | -11.121 | -11.121 | 0.000 |
| Li | 1.039e-013 | | | | |
| Li+ | 1.035e-013 | 7.702e-014 | -12.985 | -13.113 | -0.128 |
| LiSO4- | 3.448e-016 | 2.281e-016 | -15.462 | -15.642 | -0.179 |
| LiCl | 1.091e-017 | 1.091e-017 | -16.962 | -16.962 | 0.000 |
| LiOH | 3.293e-019 | 3.293e-019 | -18.482 | -18.482 | 0.000 |
| Mg | 6.467e-011 | | | | |
| MgHCO3+ | 3.890e-011 | 2.573e-011 | -10.410 | -10.590 | -0.179 |
| MgCO3 | 1.452e-011 | 1.452e-011 | -10.838 | -10.838 | 0.000 |
| Mg+2 | 1.090e-011 | 3.270e-012 | -10.963 | -11.485 | -0.523 |
| MgSO4 | 3.374e-013 | 3.374e-013 | -12.472 | -12.472 | 0.000 |
| MgCl+ | 1.817e-014 | 1.202e-014 | -13.741 | -13.920 | -0.179 |
| Mg4(OH)4+4 | 0.000e+000 | 0.000e+000 | -49.695 | -52.608 | -2.912 |
| N(-03) | 0.000e+000 | | | | |
| N3- | 0.000e+000 | 0.000e+000 | -104.277 | -104.456 | -0.179 |
| HN3 | 0.000e+000 | 0.000e+000 | -107.950 | -107.950 | 0.000 |
| N(-3) | 0.000e+000 | | | | |
| NH4+ | 0.000e+000 | 0.000e+000 | -67.676 | -67.919 | -0.243 |
| NH3 | 0.000e+000 | 0.000e+000 | -69.185 | -69.185 | 0.000 |
| NH4SO4- | 0.000e+000 | 0.000e+000 | -79.653 | -79.832 | -0.179 |
| N(0) | 1.732e-022 | | | | |
| N2 | 8.660e-023 | 8.660e-023 | -22.062 | -22.062 | 0.000 |
| N(3) | 3.621e-017 | | | | |
| NO2- | 3.621e-017 | 2.191e-017 | -16.441 | -16.659 | -0.218 |
| HNO2 | 2.385e-022 | 2.385e-022 | -21.622 | -21.622 | 0.000 |
| FeNO2+2 | 2.299e-037 | 3.690e-038 | -36.639 | -37.433 | -0.794 |
| N(5) | 8.207e-003 | | | | |

| | | | | | |
|---|---|---|---|---|---|
| NO3- | 8.206e-003 | 4.966e-003 | -2.086 | -2.304 | -0.218 |
| CaNO3+ | 2.686e-008 | 1.777e-008 | -7.571 | -7.750 | -0.179 |
| HNO3 | 1.052e-012 | 1.052e-012 | -11.978 | -11.978 | 0.000 |
| FeNO3+2 | 3.688e-025 | 5.920e-026 | -24.433 | -25.228 | -0.794 |
| Na | 1.735e-001 | | | | |
| Na+ | 9.531e-002 | 6.305e-002 | -1.021 | -1.200 | -0.179 |
| NaHCO3 | 7.564e-002 | 7.564e-002 | -1.121 | -1.121 | 0.000 |
| NaCO3- | 2.089e-003 | 1.382e-003 | -2.680 | -2.860 | -0.179 |
| NaSO4- | 3.167e-004 | 2.095e-004 | -3.499 | -3.679 | -0.179 |
| NaHSiO3 | 7.281e-005 | 7.281e-005 | -4.138 | -4.138 | 0.000 |
| NaCl | 4.764e-005 | 4.764e-005 | -4.322 | -4.322 | 0.000 |
| NaOH | 9.155e-009 | 9.155e-009 | -8.038 | -8.038 | 0.000 |
| NaAlO2 | 6.297e-014 | 6.297e-014 | -13.201 | -13.201 | 0.000 |
| O(0) | 1.841e-003 | | | | |
| O2 | 9.203e-004 | 1.209e-003 | -3.036 | -2.918 | 0.118 |
| S(-2) | 0.000e+000 | | | | |
| HS- | 0.000e+000 | 0.000e+000 | -149.104 | -149.301 | -0.197 |
| H2S | 0.000e+000 | 0.000e+000 | -150.439 | -150.439 | 0.000 |
| S-2 | 0.000e+000 | 0.000e+000 | -153.499 | -154.240 | -0.741 |
| S2-2 | 0.000e+000 | 0.000e+000 | -264.611 | -265.467 | -0.856 |
| S3-2 | 0.000e+000 | 0.000e+000 | -375.876 | -376.732 | -0.856 |
| S4-2 | 0.000e+000 | 0.000e+000 | -487.371 | -488.227 | -0.856 |
| S5-2 | 0.000e+000 | 0.000e+000 | -599.093 | -599.949 | -0.856 |
| S(2) | 0.000e+000 | | | | |
| S2O3-2 | 0.000e+000 | 0.000e+000 | -155.137 | -155.992 | -0.856 |
| HS2O3- | 0.000e+000 | 0.000e+000 | -163.088 | -163.267 | -0.179 |
| S(3) | 0.000e+000 | | | | |
| S2O4-2 | 0.000e+000 | 0.000e+000 | -140.952 | -141.693 | -0.741 |
| S(4) | 0.000e+000 | | | | |
| SO3-2 | 0.000e+000 | 0.000e+000 | -49.291 | -50.086 | -0.794 |
| HSO3- | 0.000e+000 | 0.000e+000 | -51.016 | -51.196 | -0.179 |
| H2SO3 | 0.000e+000 | 0.000e+000 | -57.449 | -57.449 | 0.000 |
| SO2 | 0.000e+000 | 0.000e+000 | -57.685 | -57.685 | 0.000 |
| S2O6-2 | 0.000e+000 | 0.000e+000 | -74.375 | -75.231 | -0.856 |
| S3O6-2 | 0.000e+000 | 0.000e+000 | -188.169 | -189.025 | -0.856 |
| S4O6-2 | 0.000e+000 | 0.000e+000 | -285.697 | -286.553 | -0.856 |
| S5O6-2 | 0.000e+000 | 0.000e+000 | -412.731 | -413.587 | -0.856 |
| S(5) | 0.000e+000 | | | | |
| S2O5-2 | 0.000e+000 | 0.000e+000 | -106.328 | -107.184 | -0.856 |
| S(6) | 7.583e-003 | | | | |
| KSO4- | 3.657e-003 | 2.419e-003 | -2.437 | -2.616 | -0.179 |
| SO4-2 | 3.610e-003 | 5.029e-004 | -2.443 | -3.299 | -0.856 |
| NaSO4- | 3.167e-004 | 2.095e-004 | -3.499 | -3.679 | -0.179 |
| CaSO4 | 4.789e-008 | 4.789e-008 | -7.320 | -7.320 | 0.000 |
| HSO4- | 2.984e-010 | 1.974e-010 | -9.525 | -9.705 | -0.179 |
| KHSO4 | 7.564e-012 | 7.564e-012 | -11.121 | -11.121 | 0.000 |
| MgSO4 | 3.374e-013 | 3.374e-013 | -12.472 | -12.472 | 0.000 |
| LiSO4- | 3.448e-016 | 2.281e-016 | -15.462 | -15.642 | -0.179 |
| AlSO4+ | 3.437e-021 | 2.274e-021 | -20.464 | -20.643 | -0.179 |
| H2SO4 | 1.270e-021 | 1.270e-021 | -20.896 | -20.896 | 0.000 |
| Al(SO4)2- | 1.342e-022 | 8.876e-023 | -21.872 | -22.052 | -0.179 |
| FeSO4 | 8.268e-026 | 8.268e-026 | -25.083 | -25.083 | 0.000 |
| FeSO4+ | 6.001e-026 | 3.970e-026 | -25.222 | -25.401 | -0.179 |
| Fe(SO4)2- | 7.455e-028 | 4.931e-028 | -27.128 | -27.307 | -0.179 |
| NH4SO4- | 0.000e+000 | 0.000e+000 | -79.653 | -79.832 | -0.179 |
| S(7) | 0.000e+000 | | | | |
| S2O8-2 | 0.000e+000 | 0.000e+000 | -47.397 | -48.253 | -0.856 |
| S(8) | 1.056e-031 | | | | |
| HSO5- | 1.056e-031 | 6.986e-032 | -30.976 | -31.156 | -0.179 |
| Si | 1.442e-003 | | | | |
| SiO2 | 1.339e-003 | 1.339e-003 | -2.873 | -2.873 | 0.000 |
| NaHSiO3 | 7.281e-005 | 7.281e-005 | -4.138 | -4.138 | 0.000 |

```
HSiO3-              3.049e-005  2.017e-005    -4.516    -4.695    -0.179
H6(H2SiO4)4-2       1.447e-008  2.015e-009    -7.840    -8.696    -0.856
H2SiO4-2            3.670e-009  5.113e-010    -8.435    -9.291    -0.856
H4(H2SiO4)4-4       1.391e-011  3.812e-015   -10.857   -14.419    -3.562
```

## File 14. Fresh Cement, Maximum Ion Content, Cement Rebar, Stainless Steel

*INPUT FILE*

```
SOLUTION 1
   temp      15
   pH        7.5
   pe        4
   redox     pe
   units     mmol/kgw
   density   1
   Alkalinity 0
   Cl(-1)    7.5
   Li        1e-010
   Al        1e-010
   Ca        3.1
   Mg        5
   Na        18
   K         1.9
   S(6)      7.3
   N(5)      7.9
   C(4)      21.8
   Br(-1)    0
   Si        0.01
   -water    1 # kg

GAS_PHASE 1
   -fixed_pressure
   -pressure 1
   -volume 1000
   -temperature 25
   CO2(g)    0.056
   O2(g)     0.18
EQUILIBRIUM_PHASES 1
   Brucite   0 1.39
   Ca(OH)2*(CSH(1.5)) 0 9.5
   Calcite   0 0.001
   CSH(1.0-2.5) 0 15.96
   Gibbsite  0 0.001
   goethite  0 1e-005
   KOH(cement) 0 0.99
   NaOH(cement) 0 0.15
   SiO2(am)  0 0.02
REACTION 1
   Fe        1
   4.75 moles in 60 steps
SAVE solution 1-1
END
USE solution 1
GAS_PHASE 2
   -fixed_volume
   -equilibrium with solution 1
   -pressure 1
   -volume 9
   -temperature 25
   CO2(g)    0.056
   O2(g)     0.18
```

```
EQUILIBRIUM_PHASES 2
   calcite   0 1e-010
   Fe(OH)3   0 1e-010
   goethite  0 1e-010
   portlandite 0 1e-010
   SiO2(am)  0 1e-010
REACTION 3
   Fe        1
   0.025 moles in 60 steps
```

## *SAMPLE OUTPUT, FINAL TIME STEP (FILE 14)*

```
Reaction step 60.

Using solution 1.       Solution after simulation 1.
Using pure phase assemblage 2.
Using gas phase 2.   Gas phase after simulation 2.
Using reaction 3.

Reaction 3.       Irreversible reaction defined in simulation 2.

      2.500e-002 moles of the following reaction have been added:

                  Relative
      Reactant          moles

      Fe               1.00000

                  Relative
      Element           moles
      Fe               1.00000

-----------------------------------Gas phase-----------------------------------


Total pressure:   0.9509   atmospheres
   Gas volume:  9.00e+000 liters

                                        Moles in gas
                                  ----------------------------------
Component              log P          P     Initial       Final       Delta

CO2(g)               -12.55  2.844e-013  1.083e-013  1.083e-013 -2.393e-017
O2(g)                -0.02  9.509e-001  3.806e-001  3.619e-001 -1.869e-002

-------------------------------Phase assemblage--------------------------------

                                        Moles in assemblage
Phase                SI log IAP  log KT      Initial       Final       Delta

Calcite            -0.00    1.98    1.98   1.000e-010  1.007e-008  9.973e-009
Fe(OH)3            -5.26    0.89    6.15   1.000e-010           0 -1.000e-010
Goethite           -0.00    0.91    0.91   1.000e-010  2.500e-002  2.500e-002
Portlandite        -1.05   22.28   23.33   1.000e-010           0 -1.000e-010
SiO2(am)           -4.60   -7.48   -2.87   1.000e-010           0 -1.000e-010

-----------------------------Solution composition------------------------------

      Elements           Molality       Moles

      Al              1.001e-003  1.000e-003
      C               1.750e-002  1.748e-002
```

| | |
|---|---|
| Ca | 4.597e-005 4.590e-005 |
| Cl | 7.510e-003 7.500e-003 |
| Fe | 3.534e-007 3.529e-007 |
| K | 9.932e-001 9.919e-001 |
| Li | 1.001e-013 1.000e-013 |
| Mg | 3.731e-011 3.726e-011 |
| N | 7.911e-003 7.900e-003 |
| Na | 1.682e-001 1.680e-001 |
| S | 7.310e-003 7.300e-003 |
| Si | 3.821e-002 3.816e-002 |

----------Description of solution----------

pH = 14.094 Charge balance
pe = 7.436 Adjusted to redox equilibrium
Activity of water = 0.965
Ionic strength = 1.007e+000
Mass of water (kg) = 9.987e-001
Total alkalinity (eq/kg) = 1.149e+000
Total CO2 (mol/kg) = 1.750e-002
Temperature (deg C) = 15.000
Electrical balance (eq) = -1.448e-002
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.76
Iterations = 5
Total H = 1.120093e+002
Total O = 5.674488e+001

----------Distribution of species----------

| Species | Molality | Log Activity | Log Molality | Log Activity | Gamma |
|---|---|---|---|---|---|
| OH- | 8.265e-001 | 5.268e-001 | -0.083 | -0.278 | -0.196 |
| H+ | 9.872e-015 | 8.060e-015 | -14.006 | -14.094 | -0.088 |
| H2O | 5.553e+001 | 9.650e-001 | 1.744 | -0.015 | 0.000 |
| Al | 1.001e-003 | | | | |
| AlO2- | 9.902e-004 | 6.559e-004 | -3.004 | -3.183 | -0.179 |
| NaAlO2 | 1.117e-005 | 1.117e-005 | -4.952 | -4.952 | 0.000 |
| HAlO2 | 2.575e-011 | 2.575e-011 | -10.589 | -10.589 | 0.000 |
| Al(OH)2+ | 4.115e-019 | 2.726e-019 | -18.386 | -18.565 | -0.179 |
| AlOH+2 | 1.159e-026 | 1.937e-027 | -25.936 | -26.713 | -0.777 |
| Al+3 | 3.723e-035 | 2.880e-036 | -34.429 | -35.541 | -1.111 |
| AlSO4+ | 2.411e-036 | 1.597e-036 | -35.618 | -35.797 | -0.179 |
| Al(SO4)2- | 1.014e-037 | 6.719e-038 | -36.994 | -37.173 | -0.179 |
| Al2(OH)2+4 | 0.000e+000 | 0.000e+000 | -47.770 | -50.615 | -2.845 |
| Al3(OH)4+5 | 0.000e+000 | 0.000e+000 | -59.970 | -64.189 | -4.219 |
| Al13O4(OH)24+7 | 0.000e+000 | 0.000e+000 | -101.886 | -110.193 | -8.308 |
| C(-2) | 0.000e+000 | | | | |
| C2H4 | 0.000e+000 | 0.000e+000 | -295.791 | -295.791 | 0.000 |
| C(-3) | 0.000e+000 | | | | |
| C2H6 | 0.000e+000 | 0.000e+000 | -267.646 | -267.646 | 0.000 |
| C(-4) | 0.000e+000 | | | | |
| CH4 | 0.000e+000 | 0.000e+000 | -164.003 | -164.003 | 0.000 |
| C(2) | 0.000e+000 | | | | |
| CO | 0.000e+000 | 0.000e+000 | -62.239 | -62.239 | 0.000 |
| C(4) | 1.750e-002 | | | | |
| CO3-2 | 1.567e-002 | 2.618e-003 | -1.805 | -2.582 | -0.777 |
| NaCO3- | 1.829e-003 | 1.212e-003 | -2.738 | -2.917 | -0.179 |
| CaCO3 | 6.322e-006 | 6.322e-006 | -5.199 | -5.199 | 0.000 |
| HCO3- | 8.856e-007 | 5.866e-007 | -6.053 | -6.232 | -0.179 |
| NaHCO3 | 1.038e-007 | 1.038e-007 | -6.984 | -6.984 | 0.000 |
| MgCO3 | 1.540e-011 | 1.540e-011 | -10.812 | -10.812 | 0.000 |

| | | | | | |
|---|---|---|---|---|---|
| CaHCO3+ | 1.366e-011 | 9.048e-012 | -10.865 | -11.043 | -0.179 |
| CO2 | 1.040e-014 | 1.318e-014 | -13.983 | -13.880 | 0.103 |
| MgHCO3+ | 6.453e-017 | 4.274e-017 | -16.190 | -16.369 | -0.179 |
| FeCO3 | 4.414e-034 | 4.414e-034 | -33.355 | -33.355 | 0.000 |
| FeCO3+ | 2.594e-034 | 1.719e-034 | -33.586 | -33.765 | -0.179 |
| FeHCO3+ | 1.119e-039 | 7.413e-040 | -38.951 | -39.130 | -0.179 |
| Ca | 4.597e-005 | | | | |
| CaOH+ | 3.371e-005 | 2.233e-005 | -4.472 | -4.651 | -0.179 |
| CaCO3 | 6.322e-006 | 6.322e-006 | -5.199 | -5.199 | 0.000 |
| Ca+2 | 5.785e-006 | 1.320e-006 | -5.238 | -5.879 | -0.642 |
| CaSO4 | 9.544e-008 | 9.544e-008 | -7.020 | -7.020 | 0.000 |
| CaNO3+ | 4.817e-008 | 3.190e-008 | -7.317 | -7.496 | -0.179 |
| CaCl+ | 1.851e-009 | 1.226e-009 | -8.733 | -8.911 | -0.179 |
| CaHCO3+ | 1.366e-011 | 9.048e-012 | -10.865 | -11.043 | -0.179 |
| CaCl2 | 7.226e-012 | 7.226e-012 | -11.141 | -11.141 | 0.000 |
| Cl(-1) | 7.510e-003 | | | | |
| Cl- | 7.376e-003 | 4.495e-003 | -2.132 | -2.347 | -0.215 |
| NaCl | 7.487e-005 | 7.487e-005 | -4.126 | -4.126 | 0.000 |
| KCl | 5.908e-005 | 5.908e-005 | -4.229 | -4.229 | 0.000 |
| CaCl+ | 1.851e-009 | 1.226e-009 | -8.733 | -8.911 | -0.179 |
| CaCl2 | 7.226e-012 | 7.226e-012 | -11.141 | -11.141 | 0.000 |
| MgCl+ | 3.452e-014 | 2.286e-014 | -13.462 | -13.641 | -0.179 |
| HCl | 7.985e-018 | 7.985e-018 | -17.098 | -17.098 | 0.000 |
| LiCl | 3.356e-018 | 3.356e-018 | -17.474 | -17.474 | 0.000 |
| FeCl+ | 1.144e-038 | 7.578e-039 | -37.942 | -38.120 | -0.179 |
| FeCl2 | 0.000e+000 | 0.000e+000 | -42.760 | -42.760 | 0.000 |
| FeCl2+ | 0.000e+000 | 0.000e+000 | -43.729 | -43.908 | -0.179 |
| FeCl+2 | 0.000e+000 | 0.000e+000 | -43.915 | -44.692 | -0.777 |
| FeCl4-2 | 0.000e+000 | 0.000e+000 | -46.164 | -47.000 | -0.835 |
| FeCl4- | 0.000e+000 | 0.000e+000 | -51.343 | -51.522 | -0.179 |
| Cl(1) | 7.956e-020 | | | | |
| ClO- | 7.956e-020 | 5.270e-020 | -19.099 | -19.278 | -0.179 |
| HClO | 1.575e-026 | 1.575e-026 | -25.803 | -25.803 | 0.000 |
| Cl(3) | 1.547e-029 | | | | |
| ClO2- | 1.547e-029 | 1.025e-029 | -28.810 | -28.989 | -0.179 |
| HClO2 | 1.221e-040 | 1.221e-040 | -39.913 | -39.913 | 0.000 |
| Cl(5) | 6.693e-025 | | | | |
| ClO3- | 6.693e-025 | 4.266e-025 | -24.174 | -24.370 | -0.196 |
| Cl(7) | 1.169e-024 | | | | |
| ClO4- | 1.169e-024 | 7.448e-025 | -23.932 | -24.128 | -0.196 |
| Fe(2) | 9.624e-025 | | | | |
| Fe(OH)3- | 6.239e-025 | 4.132e-025 | -24.205 | -24.384 | -0.179 |
| Fe(OH)4-2 | 3.384e-025 | 4.947e-026 | -24.471 | -25.306 | -0.835 |
| Fe(OH)2 | 8.670e-029 | 8.670e-029 | -28.062 | -28.062 | 0.000 |
| FeOH+ | 1.376e-031 | 9.116e-032 | -30.861 | -31.040 | -0.179 |
| FeCO3 | 4.414e-034 | 4.414e-034 | -33.355 | -33.355 | 0.000 |
| Fe+2 | 1.055e-035 | 2.408e-036 | -34.977 | -35.618 | -0.642 |
| FeSO4 | 2.068e-037 | 2.068e-037 | -36.684 | -36.684 | 0.000 |
| FeCl+ | 1.144e-038 | 7.578e-039 | -37.942 | -38.120 | -0.179 |
| FeHCO3+ | 1.119e-039 | 7.413e-040 | -38.951 | -39.130 | -0.179 |
| FeCl2 | 0.000e+000 | 0.000e+000 | -42.760 | -42.760 | 0.000 |
| FeCl4-2 | 0.000e+000 | 0.000e+000 | -46.164 | -47.000 | -0.835 |
| Fe(3) | 3.534e-007 | | | | |
| Fe(OH)4- | 3.534e-007 | 2.341e-007 | -6.452 | -6.631 | -0.179 |
| Fe(OH)3 | 7.784e-012 | 7.784e-012 | -11.109 | -11.109 | 0.000 |
| Fe(OH)2+ | 2.098e-019 | 1.390e-019 | -18.678 | -18.857 | -0.179 |
| FeOH+2 | 2.098e-029 | 3.506e-030 | -28.678 | -29.455 | -0.777 |
| FeCO3+ | 2.594e-034 | 1.719e-034 | -33.586 | -33.765 | -0.179 |
| Fe+3 | 0.000e+000 | 0.000e+000 | -40.232 | -41.343 | -1.111 |
| FeNO3+2 | 0.000e+000 | 0.000e+000 | -41.883 | -42.660 | -0.777 |
| FeSO4+ | 0.000e+000 | 0.000e+000 | -42.610 | -42.788 | -0.179 |
| FeCl2+ | 0.000e+000 | 0.000e+000 | -43.729 | -43.908 | -0.179 |

| | | | | | |
|---|---|---|---|---|---|
| FeCl+2 | 0.000e+000 | 0.000e+000 | -43.915 | -44.692 | -0.777 |
| Fe(SO4)2- | 0.000e+000 | 0.000e+000 | -44.483 | -44.662 | -0.179 |
| FeCl4- | 0.000e+000 | 0.000e+000 | -51.343 | -51.522 | -0.179 |
| FeNO2+2 | 0.000e+000 | 0.000e+000 | -54.130 | -54.907 | -0.777 |
| Fe2(OH)2+4 | 0.000e+000 | 0.000e+000 | -54.635 | -57.480 | -2.845 |
| Fe3(OH)4+5 | 0.000e+000 | 0.000e+000 | -69.798 | -74.017 | -4.219 |
| H(0) | 0.000e+000 | | | | |
| H2 | 0.000e+000 | 0.000e+000 | -46.470 | -46.368 | 0.103 |
| K | 9.932e-001 | | | | |
| K+ | 7.902e-001 | 4.816e-001 | -0.102 | -0.317 | -0.215 |
| KOH | 1.999e-001 | 1.999e-001 | -0.699 | -0.699 | 0.000 |
| KSO4- | 3.050e-003 | 2.021e-003 | -2.516 | -2.695 | -0.179 |
| KCl | 5.908e-005 | 5.908e-005 | -4.229 | -4.229 | 0.000 |
| KHSO4 | 9.893e-018 | 9.893e-018 | -17.005 | -17.005 | 0.000 |
| Li | 1.001e-013 | | | | |
| LiOH | 6.702e-014 | 6.702e-014 | -13.174 | -13.174 | 0.000 |
| Li+ | 3.300e-014 | 2.443e-014 | -13.481 | -13.612 | -0.131 |
| LiSO4- | 1.177e-016 | 7.797e-017 | -15.929 | -16.108 | -0.179 |
| LiCl | 3.356e-018 | 3.356e-018 | -17.474 | -17.474 | 0.000 |
| Mg | 3.731e-011 | | | | |
| Mg+2 | 2.116e-011 | 6.417e-012 | -10.675 | -11.193 | -0.518 |
| MgCO3 | 1.540e-011 | 1.540e-011 | -10.812 | -10.812 | 0.000 |
| MgSO4 | 7.133e-013 | 7.133e-013 | -12.147 | -12.147 | 0.000 |
| MgCl+ | 3.452e-014 | 2.286e-014 | -13.462 | -13.641 | -0.179 |
| MgHCO3+ | 6.453e-017 | 4.274e-017 | -16.190 | -16.369 | -0.179 |
| Mg4(OH)4+4 | 4.338e-026 | 6.194e-029 | -25.363 | -28.208 | -2.845 |
| N(-03) | 0.000e+000 | | | | |
| N3- | 0.000e+000 | 0.000e+000 | -116.262 | -116.441 | -0.179 |
| HN3 | 0.000e+000 | 0.000e+000 | -125.740 | -125.740 | 0.000 |
| N(-3) | 0.000e+000 | | | | |
| NH3 | 0.000e+000 | 0.000e+000 | -75.169 | -75.169 | 0.000 |
| NH4+ | 0.000e+000 | 0.000e+000 | -79.469 | -79.707 | -0.238 |
| NH4SO4- | 0.000e+000 | 0.000e+000 | -91.409 | -91.588 | -0.179 |
| N(0) | 2.463e-034 | | | | |
| N2 | 1.232e-034 | 1.232e-034 | -33.910 | -33.910 | 0.000 |
| N(3) | 3.171e-017 | | | | |
| NO2- | 3.171e-017 | 1.932e-017 | -16.499 | -16.714 | -0.215 |
| HNO2 | 3.293e-028 | 3.293e-028 | -27.482 | -27.482 | 0.000 |
| FeNO2+2 | 0.000e+000 | 0.000e+000 | -54.130 | -54.907 | -0.777 |
| N(5) | 7.911e-003 | | | | |
| NO3- | 7.911e-003 | 4.821e-003 | -2.102 | -2.317 | -0.215 |
| CaNO3+ | 4.817e-008 | 3.190e-008 | -7.317 | -7.496 | -0.179 |
| HNO3 | 1.598e-018 | 1.598e-018 | -17.796 | -17.796 | 0.000 |
| FeNO3+2 | 0.000e+000 | 0.000e+000 | -41.883 | -42.660 | -0.777 |
| Na | 1.682e-001 | | | | |
| Na+ | 1.543e-001 | 1.022e-001 | -0.811 | -0.990 | -0.179 |
| NaOH | 9.523e-003 | 9.523e-003 | -2.021 | -2.021 | 0.000 |
| NaHSiO3 | 1.886e-003 | 1.886e-003 | -2.724 | -2.724 | 0.000 |
| NaCO3- | 1.829e-003 | 1.212e-003 | -2.738 | -2.917 | -0.179 |
| NaSO4- | 5.526e-004 | 3.661e-004 | -3.258 | -3.436 | -0.179 |
| NaCl | 7.487e-005 | 7.487e-005 | -4.126 | -4.126 | 0.000 |
| NaAlO2 | 1.117e-005 | 1.117e-005 | -4.952 | -4.952 | 0.000 |
| NaHCO3 | 1.038e-007 | 1.038e-007 | -6.984 | -6.984 | 0.000 |
| O(0) | 2.313e-003 | | | | |
| O2 | 1.156e-003 | 1.465e-003 | -2.937 | -2.834 | 0.103 |
| S(-2) | 0.000e+000 | | | | |
| S-2 | 0.000e+000 | 0.000e+000 | -153.648 | -154.374 | -0.726 |
| HS- | 0.000e+000 | 0.000e+000 | -155.046 | -155.241 | -0.196 |
| H2S | 0.000e+000 | 0.000e+000 | -162.184 | -162.184 | 0.000 |
| S2-2 | 0.000e+000 | 0.000e+000 | -276.472 | -277.307 | -0.835 |
| S3-2 | 0.000e+000 | 0.000e+000 | -399.442 | -400.277 | -0.835 |
| S4-2 | 0.000e+000 | 0.000e+000 | -522.643 | -523.478 | -0.835 |

```
  S5-2              0.000e+000  0.000e+000  -646.070  -646.905    -0.835
S(2)          0.000e+000
  S2O3-2            0.000e+000  0.000e+000  -166.872  -167.707    -0.835
  HS2O3-            0.000e+000  0.000e+000  -180.608  -180.787    -0.179
S(3)          0.000e+000
  S2O4-2            0.000e+000  0.000e+000  -152.639  -153.366    -0.726
S(4)          0.000e+000
  SO3-2             0.000e+000  0.000e+000   -49.318   -50.095    -0.777
  HSO3-             0.000e+000  0.000e+000   -56.831   -57.010    -0.179
  H2SO3             0.000e+000  0.000e+000   -69.069   -69.069     0.000
  SO2               0.000e+000  0.000e+000   -69.307   -69.307     0.000
  S2O6-2            0.000e+000  0.000e+000   -85.986   -86.821    -0.835
  S3O6-2            0.000e+000  0.000e+000  -211.484  -212.320    -0.835
  S4O6-2            0.000e+000  0.000e+000  -320.718  -321.553    -0.835
  S5O6-2            0.000e+000  0.000e+000  -459.457  -460.292    -0.835
S(5)          0.000e+000
  S2O5-2            0.000e+000  0.000e+000  -117.980  -118.815    -0.835
S(6)          7.310e-003
  SO4-2             3.707e-003  5.419e-004    -2.431    -3.266    -0.835
  KSO4-             3.050e-003  2.021e-003    -2.516    -2.695    -0.179
  NaSO4-            5.526e-004  3.661e-004    -3.258    -3.436    -0.179
  CaSO4             9.544e-008  9.544e-008    -7.020    -7.020     0.000
  MgSO4             7.133e-013  7.133e-013   -12.147   -12.147     0.000
  HSO4-             5.028e-016  3.330e-016   -15.299   -15.477    -0.179
  LiSO4-            1.177e-016  7.797e-017   -15.929   -16.108    -0.179
  KHSO4             9.893e-018  9.893e-018   -17.005   -17.005     0.000
  H2SO4             3.355e-033  3.355e-033   -32.474   -32.474     0.000
  AlSO4+            2.411e-036  1.597e-036   -35.618   -35.797    -0.179
  FeSO4             2.068e-037  2.068e-037   -36.684   -36.684     0.000
  Al(SO4)2-         1.014e-037  6.719e-038   -36.994   -37.173    -0.179
  FeSO4+            0.000e+000  0.000e+000   -42.610   -42.788    -0.179
  Fe(SO4)2-         0.000e+000  0.000e+000   -44.483   -44.662    -0.179
  NH4SO4-           0.000e+000  0.000e+000   -91.409   -91.588    -0.179
S(7)          0.000e+000
  S2O8-2            0.000e+000  0.000e+000   -58.924   -59.759    -0.835
S(8)          1.959e-037
  HSO5-             1.959e-037  1.298e-037   -36.708   -36.887    -0.179
Si            3.821e-002
  H2SiO4-2          3.584e-002  5.239e-003    -1.446    -2.281    -0.835
  NaHSiO3           1.886e-003  1.886e-003    -2.724    -2.724     0.000
  HSiO3-            4.864e-004  3.222e-004    -3.313    -3.492    -0.179
  H4(H2SiO4)4-4     7.281e-007  2.526e-010    -6.138    -9.598    -3.460
  SiO2              3.334e-008  3.334e-008    -7.477    -7.477     0.000
  H6(H2SiO4)4-2     2.239e-015  3.274e-016   -14.650   -15.485    -0.835
```

## File 15. Mature Cement, Minimum Ion Content, Cement Rebar, Carbon Steel

*INPUT FILE*

```
SOLUTION 1
    temp      15
    pH        7.5
    pe        4
    redox     pe
    units     mmol/kgw
    density   1
    Alkalinity 0
    Cl(-1)    0
    Li        1e-010
    Al        1e-010
    Ca        0.6
    Mg        0.3
```

```
    Na       1.3
    K        0
    S(6)     0.3
    N(5)     0
    C(4)     1.4
    Br(-1)   0
    Si       0.01
    -water   1 # kg

GAS_PHASE 1
    -fixed_pressure
    -pressure 1
    -volume 1000
    -temperature 25
    CO2(g)   0.056
    O2(g)    0.18
EQUILIBRIUM_PHASES 1
    Brucite   0 1.39
    Ca(OH)2*(CSH(1.5)) 0 9.5
    Calcite   0 0.001
    CSH(1.0-2.5) 0 15.96
    Gibbsite  0 0.001
    goethite  0 1e-005
    SiO2(am)  0 0.02
REACTION 1
    Fe       1
    4.75 moles in 60 steps
SAVE solution 1-1
END
USE solution 1
GAS_PHASE 2
    -fixed_pressure
    -pressure 1
    -volume 1000
    -temperature 25
    CO2(g)   0.056
    O2(g)    0.18
EQUILIBRIUM_PHASES 2
    calcite   0 1e-010
    Fe(OH)3   0 1e-010
    goethite  0 1e-010
    portlandite 0 1e-010
    SiO2(am)  0 1e-010
REACTION 3
    Fe       1
    4.05 moles in 60 steps
```

## *SAMPLE OUTPUT, FINAL TIME STEP (FILE 15)*

```
Reaction step 60.

Using solution 1.       Solution after simulation 1.
Using pure phase assemblage 2.
Using gas phase 2.
Using reaction 3.

Reaction 3.       Irreversible reaction defined in simulation 2.

      4.050e+000 moles of the following reaction have been added:

                  Relative
      Reactant          moles
```

```
      Fe                1.00000

                    Relative
      Element           moles
      Fe                1.00000

-----------------------------------Gas phase------------------------------------


Total pressure:   1.0000   atmospheres
   Gas volume:  1.56e+002 liters

                                        Moles in gas
                                    ---------------------------------
Component             log P          P     Initial       Final       Delta

CO2(g)                -0.46  3.434e-001  2.289e+000  2.260e+000 -2.930e-002
O2(g)                 -0.18  6.566e-001  7.357e+000  4.320e+000 -3.037e+000

--------------------------------Phase assemblage--------------------------------

                                        Moles in assemblage
Phase               SI log IAP  log KT      Initial       Final       Delta

Calcite           -0.00    1.98    1.98   1.000e-010  1.087e-005  1.087e-005
Fe(OH)3           -5.25    0.91    6.15   1.000e-010           0 -1.000e-010
Goethite          -0.00    0.91    0.91   1.000e-010  4.050e+000  4.050e+000
Portlandite      -13.12   10.21   23.33   1.000e-010           0 -1.000e-010
SiO2(am)          -2.07   -4.94   -2.87   1.000e-010           0 -1.000e-010

-----------------------------Solution composition-----------------------------

      Elements          Molality       Moles

      Al             6.642e-004  6.390e-004
      C              3.046e-002  2.930e-002
      Ca             7.401e-003  7.120e-003
      Fe             1.786e-011  1.718e-011
      Li             1.039e-013  1.000e-013
      Mg             2.858e-008  2.750e-008
      Na             1.351e-003  1.300e-003
      S              3.118e-004  3.000e-004
      Si             1.151e-005  1.107e-005

----------------------------Description of solution----------------------------

                                pH  =   6.310      Charge balance
                                pe  =  15.171      Adjusted to redox equilibrium
                     Activity of water  =   0.999
                        Ionic strength  =  2.308e-002
                     Mass of water (kg)  =  9.620e-001
                Total alkalinity (eq/kg)  =  1.628e-002
                     Total CO2 (mol/kg)  =  3.046e-002
                    Temperature (deg C)  =  15.000
                Electrical balance (eq)  =  1.199e-003
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   4.13
                           Iterations  =  18
                             Total H  = 1.068469e+002
                             Total O  = 5.349302e+001

----------------------------Distribution of species----------------------------
```

| Species | Molality | Log Activity | Log Molality | Log Activity | Gamma |
|---|---|---|---|---|---|
| H+ | 5.516e-007 | 4.894e-007 | -6.258 | -6.310 | -0.052 |
| OH- | 1.042e-008 | 8.985e-009 | -7.982 | -8.046 | -0.064 |
| H2O | 5.553e+001 | 9.993e-001 | 1.744 | -0.000 | 0.000 |
| Al | 6.642e-004 | | | | |
| Al13O4(OH)24+7 | 5.106e-005 | 6.564e-008 | -4.292 | -7.183 | -2.891 |
| HAlO2 | 1.385e-007 | 1.385e-007 | -6.859 | -6.859 | 0.000 |
| Al(OH)2+ | 1.029e-007 | 8.898e-008 | -6.988 | -7.051 | -0.063 |
| AlO2- | 6.715e-008 | 5.808e-008 | -7.173 | -7.236 | -0.063 |
| AlOH+2 | 6.584e-008 | 3.707e-008 | -7.181 | -7.431 | -0.250 |
| Al+3 | 9.660e-009 | 3.232e-009 | -8.015 | -8.491 | -0.475 |
| AlSO4+ | 5.127e-010 | 4.435e-010 | -9.290 | -9.353 | -0.063 |
| NaAlO2 | 1.110e-011 | 1.110e-011 | -10.955 | -10.955 | 0.000 |
| Al2(OH)2+4 | 8.143e-012 | 8.891e-013 | -11.089 | -12.051 | -0.962 |
| Al(SO4)2- | 5.336e-012 | 4.616e-012 | -11.273 | -11.336 | -0.063 |
| Al3(OH)4+5 | 2.307e-013 | 7.736e-015 | -12.637 | -14.111 | -1.475 |
| C(-2) | 0.000e+000 | | | | |
| C2H4 | 0.000e+000 | 0.000e+000 | -271.114 | -271.114 | 0.000 |
| C(-3) | 0.000e+000 | | | | |
| C2H6 | 0.000e+000 | 0.000e+000 | -242.874 | -242.874 | 0.000 |
| C(-4) | 0.000e+000 | | | | |
| CH4 | 0.000e+000 | 0.000e+000 | -151.569 | -151.569 | 0.000 |
| C(2) | 0.000e+000 | | | | |
| CO | 0.000e+000 | 0.000e+000 | -50.077 | -50.077 | 0.000 |
| C(4) | 3.046e-002 | | | | |
| CO2 | 1.582e-002 | 1.591e-002 | -1.801 | -1.798 | 0.002 |
| HCO3- | 1.397e-002 | 1.208e-002 | -1.855 | -1.918 | -0.063 |
| CaHCO3+ | 6.351e-004 | 5.494e-004 | -3.197 | -3.260 | -0.063 |
| NaHCO3 | 2.399e-005 | 2.399e-005 | -4.620 | -4.620 | 0.000 |
| CaCO3 | 6.322e-006 | 6.322e-006 | -5.199 | -5.199 | 0.000 |
| CO3-2 | 1.577e-006 | 8.879e-007 | -5.802 | -6.052 | -0.250 |
| NaCO3- | 5.331e-009 | 4.611e-009 | -8.273 | -8.336 | -0.063 |
| MgHCO3+ | 2.463e-009 | 2.131e-009 | -8.608 | -8.671 | -0.063 |
| MgCO3 | 1.265e-011 | 1.265e-011 | -10.898 | -10.898 | 0.000 |
| FeCO3+ | 1.406e-014 | 1.217e-014 | -13.852 | -13.915 | -0.063 |
| FeHCO3+ | 6.773e-020 | 5.858e-020 | -19.169 | -19.232 | -0.063 |
| FeCO3 | 5.746e-022 | 5.746e-022 | -21.241 | -21.241 | 0.000 |
| Ca | 7.401e-003 | | | | |
| Ca+2 | 6.690e-003 | 3.893e-003 | -2.175 | -2.410 | -0.235 |
| CaHCO3+ | 6.351e-004 | 5.494e-004 | -3.197 | -3.260 | -0.063 |
| CaSO4 | 6.962e-005 | 6.962e-005 | -4.157 | -4.157 | 0.000 |
| CaCO3 | 6.322e-006 | 6.322e-006 | -5.199 | -5.199 | 0.000 |
| CaOH+ | 1.298e-009 | 1.123e-009 | -8.887 | -8.950 | -0.063 |
| Fe(2) | 8.438e-020 | | | | |
| FeHCO3+ | 6.773e-020 | 5.858e-020 | -19.169 | -19.232 | -0.063 |
| Fe+2 | 1.588e-020 | 9.240e-021 | -19.799 | -20.034 | -0.235 |
| FeCO3 | 5.746e-022 | 5.746e-022 | -21.241 | -21.241 | 0.000 |
| FeSO4 | 1.963e-022 | 1.963e-022 | -21.707 | -21.707 | 0.000 |
| FeOH+ | 6.898e-024 | 5.967e-024 | -23.161 | -23.224 | -0.063 |
| Fe(OH)2 | 9.679e-029 | 9.679e-029 | -28.014 | -28.014 | 0.000 |
| Fe(OH)3- | 9.097e-033 | 7.869e-033 | -32.041 | -32.104 | -0.063 |
| Fe(OH)4-2 | 0.000e+000 | 0.000e+000 | -40.539 | -40.794 | -0.255 |
| Fe(3) | 1.786e-011 | | | | |
| Fe(OH)2+ | 9.757e-012 | 8.440e-012 | -11.011 | -11.074 | -0.063 |
| Fe(OH)3 | 8.061e-012 | 8.061e-012 | -11.094 | -11.094 | 0.000 |
| FeOH+2 | 2.217e-014 | 1.248e-014 | -13.654 | -13.904 | -0.250 |
| FeCO3+ | 1.406e-014 | 1.217e-014 | -13.852 | -13.915 | -0.063 |
| Fe(OH)4- | 4.781e-015 | 4.135e-015 | -14.321 | -14.384 | -0.063 |
| Fe+3 | 2.829e-018 | 9.466e-019 | -17.548 | -18.024 | -0.475 |

| | | | | | |
|---|---|---|---|---|---|
| FeSO4+ | 9.717e-021 | 8.405e-021 | -20.012 | -20.075 | -0.063 |
| Fe(SO4)2- | 3.218e-023 | 2.784e-023 | -22.492 | -22.555 | -0.063 |
| Fe2(OH)2+4 | 3.840e-026 | 4.193e-027 | -25.416 | -26.378 | -0.962 |
| Fe3(OH)4+5 | 2.205e-034 | 7.393e-036 | -33.657 | -35.131 | -1.475 |
| H(0) | 0.000e+000 | | | | |
| H2 | 0.000e+000 | 0.000e+000 | -46.274 | -46.272 | 0.002 |
| Li | 1.039e-013 | | | | |
| Li+ | 1.039e-013 | 9.086e-014 | -12.984 | -13.042 | -0.058 |
| LiSO4- | 8.293e-017 | 7.174e-017 | -16.081 | -16.144 | -0.063 |
| LiOH | 4.251e-021 | 4.251e-021 | -20.372 | -20.372 | 0.000 |
| Mg | 2.858e-008 | | | | |
| Mg+2 | 2.568e-008 | 1.553e-008 | -7.590 | -7.809 | -0.218 |
| MgHCO3+ | 2.463e-009 | 2.131e-009 | -8.608 | -8.671 | -0.063 |
| MgSO4 | 4.272e-010 | 4.272e-010 | -9.369 | -9.369 | 0.000 |
| MgCO3 | 1.265e-011 | 1.265e-011 | -10.898 | -10.898 | 0.000 |
| Mg4(OH)4+4 | 0.000e+000 | 0.000e+000 | -44.783 | -45.745 | -0.962 |
| Na | 1.351e-003 | | | | |
| Na+ | 1.326e-003 | 1.147e-003 | -2.877 | -2.940 | -0.063 |
| NaHCO3 | 2.399e-005 | 2.399e-005 | -4.620 | -4.620 | 0.000 |
| NaSO4- | 1.175e-006 | 1.016e-006 | -5.930 | -5.993 | -0.063 |
| NaCO3- | 5.331e-009 | 4.611e-009 | -8.273 | -8.336 | -0.063 |
| NaHSiO3 | 1.246e-010 | 1.246e-010 | -9.905 | -9.905 | 0.000 |
| NaAlO2 | 1.110e-011 | 1.110e-011 | -10.955 | -10.955 | 0.000 |
| NaOH | 1.822e-012 | 1.822e-012 | -11.739 | -11.739 | 0.000 |
| O(0) | 2.012e-003 | | | | |
| O2 | 1.006e-003 | 1.012e-003 | -2.997 | -2.995 | 0.002 |
| S(-2) | 0.000e+000 | | | | |
| H2S | 0.000e+000 | 0.000e+000 | -146.903 | -146.903 | 0.000 |
| HS- | 0.000e+000 | 0.000e+000 | -147.679 | -147.743 | -0.064 |
| S-2 | 0.000e+000 | 0.000e+000 | -154.415 | -154.659 | -0.245 |
| S2-2 | 0.000e+000 | 0.000e+000 | -262.151 | -262.406 | -0.255 |
| S3-2 | 0.000e+000 | 0.000e+000 | -369.935 | -370.190 | -0.255 |
| S4-2 | 0.000e+000 | 0.000e+000 | -477.950 | -478.205 | -0.255 |
| S5-2 | 0.000e+000 | 0.000e+000 | -586.191 | -586.445 | -0.255 |
| S(2) | 0.000e+000 | | | | |
| S2O3-2 | 0.000e+000 | 0.000e+000 | -152.792 | -153.047 | -0.255 |
| HS2O3- | 0.000e+000 | 0.000e+000 | -158.281 | -158.344 | -0.063 |
| S(3) | 0.000e+000 | | | | |
| S2O4-2 | 0.000e+000 | 0.000e+000 | -138.542 | -138.786 | -0.245 |
| S(4) | 0.000e+000 | | | | |
| HSO3- | 0.000e+000 | 0.000e+000 | -49.690 | -49.753 | -0.063 |
| SO3-2 | 0.000e+000 | 0.000e+000 | -50.372 | -50.621 | -0.250 |
| H2SO3 | 0.000e+000 | 0.000e+000 | -54.029 | -54.029 | 0.000 |
| SO2 | 0.000e+000 | 0.000e+000 | -54.282 | -54.282 | 0.000 |
| S2O6-2 | 0.000e+000 | 0.000e+000 | -72.147 | -72.402 | -0.255 |
| S3O6-2 | 0.000e+000 | 0.000e+000 | -182.460 | -182.715 | -0.255 |
| S4O6-2 | 0.000e+000 | 0.000e+000 | -276.507 | -276.762 | -0.255 |
| S5O6-2 | 0.000e+000 | 0.000e+000 | -400.060 | -400.315 | -0.255 |
| S(5) | 0.000e+000 | | | | |
| S2O5-2 | 0.000e+000 | 0.000e+000 | -104.061 | -104.316 | -0.255 |
| S(6) | 3.118e-004 | | | | |
| SO4-2 | 2.411e-004 | 1.341e-004 | -3.618 | -3.873 | -0.255 |
| CaSO4 | 6.962e-005 | 6.962e-005 | -4.157 | -4.157 | 0.000 |
| NaSO4- | 1.175e-006 | 1.016e-006 | -5.930 | -5.993 | -0.063 |
| HSO4- | 5.784e-009 | 5.003e-009 | -8.238 | -8.301 | -0.063 |
| AlSO4+ | 5.127e-010 | 4.435e-010 | -9.290 | -9.353 | -0.063 |
| MgSO4 | 4.272e-010 | 4.272e-010 | -9.369 | -9.369 | 0.000 |
| Al(SO4)2- | 5.336e-012 | 4.616e-012 | -11.273 | -11.336 | -0.063 |
| LiSO4- | 8.293e-017 | 7.174e-017 | -16.081 | -16.144 | -0.063 |
| H2SO4 | 3.060e-018 | 3.060e-018 | -17.514 | -17.514 | 0.000 |
| FeSO4+ | 9.717e-021 | 8.405e-021 | -20.012 | -20.075 | -0.063 |
| FeSO4 | 1.963e-022 | 1.963e-022 | -21.707 | -21.707 | 0.000 |

```
   Fe(SO4)2-          3.218e-023  2.784e-023   -22.492   -22.555    -0.063
S(7)          0.000e+000
   S2O8-2             0.000e+000  0.000e+000   -45.246   -45.501    -0.255
S(8)          1.873e-030
   HSO5-              1.873e-030  1.620e-030   -29.727   -29.790    -0.063
Si            1.151e-005
   SiO2               1.151e-005  1.151e-005    -4.939    -4.939     0.000
   HSiO3-             2.193e-009  1.897e-009    -8.659    -8.722    -0.063
   NaHSiO3            1.246e-010  1.246e-010    -9.905    -9.905     0.000
   H2SiO4-2           9.459e-016  5.262e-016   -15.024   -15.279    -0.255
   H6(H2SiO4)4-2      2.999e-021  1.668e-021   -20.523   -20.778    -0.255
   H4(H2SiO4)4-4      3.670e-030  3.491e-031   -29.435   -30.457    -1.022
```

## File 16. Mature Cement, Minimum Ion Content, Cement Rebar, Stainless Steel

*INPUT FILE*

```
SOLUTION 1
   temp      15
   pH        7.5
   pe        4
   redox     pe
   units     mmol/kgw
   density   1
   Alkalinity 0
   Cl(-1)    0
   Li        1e-010
   Al        1e-010
   Ca        0.6
   Mg        0.3
   Na        1.3
   K         0
   S(6)      0.3
   N(5)      0
   C(4)      1.4
   Br(-1)    0
   Si        0.01
   -water    1 # kg

GAS_PHASE 1
   -fixed_pressure
   -pressure 1
   -volume 1000
   -temperature 25
   CO2(g)    0.056
   O2(g)     0.18
EQUILIBRIUM_PHASES 1
   Brucite   0 1.39
   Ca(OH)2*(CSH(1.5)) 0 9.5
   Calcite   0 0.001
   CSH(1.0-2.5) 0 15.96
   Gibbsite  0 0.001
   goethite  0 1e-005
   SiO2(am)  0 0.02
REACTION 1
   Fe        1
   4.75 moles in 60 steps
SAVE solution 1-1
END
USE solution 1
GAS_PHASE 2
   -fixed_pressure
```

```
   -pressure 1
   -volume 1000
   -temperature 25
   CO2(g)    0.056
   O2(g)     0.18
EQUILIBRIUM_PHASES 2
   calcite   0 1e-010
   Fe(OH)3   0 1e-010
   goethite  0 1e-010
   portlandite 0 1e-010
   SiO2(am)  0 1e-010
REACTION 3
   Fe        1
   0.025 moles in 60 steps
```

*SAMPLE OUTPUT, FINAL TIME STEP (FILE 16)*

```
Reaction step 60.

Using solution 1.       Solution after simulation 1.
Using pure phase assemblage 2.
Using gas phase 2.
Using reaction 3.

Reaction 3.       Irreversible reaction defined in simulation 2.

      2.500e-002 moles of the following reaction have been added:

                  Relative
      Reactant          moles

      Fe                1.00000

                  Relative
      Element           moles
      Fe                1.00000

-----------------------------------Gas phase-----------------------------------


Total pressure:   1.0000   atmospheres
   Gas volume:  2.27e+002 liters

                                          Moles in gas
                                  ----------------------------------
Component             log P          P     Initial       Final       Delta

CO2(g)                -0.63  2.358e-001  2.289e+000  2.265e+000 -2.421e-002
O2(g)                 -0.12  7.642e-001  7.357e+000  7.339e+000 -1.839e-002

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
Phase               SI log IAP  log KT      Initial       Final       Delta

Calcite           -0.00    1.98    1.98   1.000e-010  7.322e-004  7.322e-004
Fe(OH)3           -5.25    0.91    6.15   1.000e-010           0 -1.000e-010
Goethite           0.00    0.91    0.91   1.000e-010  2.500e-002  2.500e-002
Portlandite      -12.96   10.37   23.33   1.000e-010           0 -1.000e-010
SiO2(am)          -2.08   -4.96   -2.87   1.000e-010           0 -1.000e-010

----------------------------Solution composition-----------------------------
```

| Elements | Molality | Moles |
|---|---|---|
| Al | 6.401e-004 | 6.390e-004 |
| C | 2.353e-002 | 2.349e-002 |
| Ca | 6.410e-003 | 6.399e-003 |
| Fe | 1.569e-011 | 1.566e-011 |
| Li | 1.002e-013 | 1.000e-013 |
| Mg | 2.755e-008 | 2.750e-008 |
| Na | 1.302e-003 | 1.300e-003 |
| S | 3.005e-004 | 3.000e-004 |
| Si | 1.109e-005 | 1.107e-005 |

----------Description of solution----------

pH = 6.416 Charge balance
pe = 15.082 Adjusted to redox equilibrium
Activity of water = 0.999
Ionic strength = 2.033e-002
Mass of water (kg) = 9.983e-001
Total alkalinity (eq/kg) = 1.424e-002
Total CO2 (mol/kg) = 2.353e-002
Temperature (deg C) = 15.000
Electrical balance (eq) = 1.199e-003
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 4.55
Iterations = 33
Total H = 1.108719e+002
Total O = 5.549358e+001

----------Distribution of species----------

| Species | Molality | Log Activity | Log Molality | Log Activity | Gamma |
|---|---|---|---|---|---|
| H+ | 4.307e-007 | 3.840e-007 | -6.366 | -6.416 | -0.050 |
| OH- | 1.318e-008 | 1.145e-008 | -7.880 | -7.941 | -0.061 |
| H2O | 5.553e+001 | 9.995e-001 | 1.744 | -0.000 | 0.000 |
| Al | 6.401e-004 | | | | |
| Al13O4(OH)24+7 | 4.921e-005 | 8.709e-008 | -4.308 | -7.060 | -2.752 |
| HAlO2 | 1.612e-007 | 1.612e-007 | -6.793 | -6.793 | 0.000 |
| AlO2- | 9.891e-008 | 8.619e-008 | -7.005 | -7.065 | -0.060 |
| Al(OH)2+ | 9.331e-008 | 8.131e-008 | -7.030 | -7.090 | -0.060 |
| AlOH+2 | 4.586e-008 | 2.658e-008 | -7.339 | -7.576 | -0.237 |
| Al+3 | 5.184e-009 | 1.818e-009 | -8.285 | -8.740 | -0.455 |
| AlSO4+ | 2.893e-010 | 2.521e-010 | -9.539 | -9.598 | -0.060 |
| NaAlO2 | 1.603e-011 | 1.603e-011 | -10.795 | -10.795 | 0.000 |
| Al2(OH)2+4 | 3.756e-012 | 4.571e-013 | -11.425 | -12.340 | -0.915 |
| Al(SO4)2- | 3.042e-012 | 2.651e-012 | -11.517 | -11.577 | -0.060 |
| Al3(OH)4+5 | 9.207e-014 | 3.634e-015 | -13.036 | -14.440 | -1.404 |
| C(-2) | 0.000e+000 | | | | |
| C2H4 | 0.000e+000 | 0.000e+000 | -271.638 | -271.638 | 0.000 |
| C(-3) | 0.000e+000 | | | | |
| C2H6 | 0.000e+000 | 0.000e+000 | -243.430 | -243.430 | 0.000 |
| C(-4) | 0.000e+000 | | | | |
| CH4 | 0.000e+000 | 0.000e+000 | -151.864 | -151.864 | 0.000 |
| C(2) | 0.000e+000 | | | | |
| CO | 0.000e+000 | 0.000e+000 | -50.273 | -50.273 | 0.000 |
| C(4) | 2.353e-002 | | | | |
| HCO3- | 1.213e-002 | 1.057e-002 | -1.916 | -1.976 | -0.060 |
| CO2 | 1.087e-002 | 1.093e-002 | -1.964 | -1.961 | 0.002 |
| CaHCO3+ | 4.948e-004 | 4.311e-004 | -3.306 | -3.365 | -0.060 |
| NaHCO3 | 2.043e-005 | 2.043e-005 | -4.690 | -4.690 | 0.000 |

| | | | | | |
|---|---|---|---|---|---|
| CaCO3 | 6.322e-006 | 6.322e-006 | -5.199 | -5.199 | 0.000 |
| CO3-2 | 1.709e-006 | 9.902e-007 | -5.767 | -6.004 | -0.237 |
| NaCO3- | 5.741e-009 | 5.003e-009 | -8.241 | -8.301 | -0.060 |
| MgHCO3+ | 2.128e-009 | 1.855e-009 | -8.672 | -8.732 | -0.060 |
| MgCO3 | 1.403e-011 | 1.403e-011 | -10.853 | -10.853 | 0.000 |
| FeCO3+ | 7.523e-015 | 6.555e-015 | -14.124 | -14.183 | -0.060 |
| FeHCO3+ | 3.488e-020 | 3.039e-020 | -19.457 | -19.517 | -0.060 |
| FeCO3 | 3.798e-022 | 3.798e-022 | -21.420 | -21.420 | 0.000 |
| Ca | 6.410e-003 | | | | |
| Ca+2 | 5.846e-003 | 3.491e-003 | -2.233 | -2.457 | -0.224 |
| CaHCO3+ | 4.948e-004 | 4.311e-004 | -3.306 | -3.365 | -0.060 |
| CaSO4 | 6.307e-005 | 6.307e-005 | -4.200 | -4.200 | 0.000 |
| CaCO3 | 6.322e-006 | 6.322e-006 | -5.199 | -5.199 | 0.000 |
| CaOH+ | 1.473e-009 | 1.283e-009 | -8.832 | -8.892 | -0.060 |
| Fe(2) | 4.455e-020 | | | | |
| FeHCO3+ | 3.488e-020 | 3.039e-020 | -19.457 | -19.517 | -0.060 |
| Fe+2 | 9.172e-021 | 5.477e-021 | -20.038 | -20.261 | -0.224 |
| FeCO3 | 3.798e-022 | 3.798e-022 | -21.420 | -21.420 | 0.000 |
| FeSO4 | 1.176e-022 | 1.176e-022 | -21.930 | -21.930 | 0.000 |
| FeOH+ | 5.173e-024 | 4.508e-024 | -23.286 | -23.346 | -0.060 |
| Fe(OH)2 | 9.319e-029 | 9.319e-029 | -28.031 | -28.031 | 0.000 |
| Fe(OH)3- | 1.108e-032 | 9.656e-033 | -31.955 | -32.015 | -0.060 |
| Fe(OH)4-2 | 0.000e+000 | 0.000e+000 | -40.358 | -40.600 | -0.242 |
| Fe(3) | 1.569e-011 | | | | |
| Fe(OH)3 | 8.062e-012 | 8.062e-012 | -11.094 | -11.094 | 0.000 |
| Fe(OH)2+ | 7.601e-012 | 6.623e-012 | -11.119 | -11.179 | -0.060 |
| FeOH+2 | 1.326e-014 | 7.685e-015 | -13.877 | -14.114 | -0.237 |
| FeCO3+ | 7.523e-015 | 6.555e-015 | -14.124 | -14.183 | -0.060 |
| Fe(OH)4- | 6.049e-015 | 5.271e-015 | -14.218 | -14.278 | -0.060 |
| Fe+3 | 1.304e-018 | 4.573e-019 | -17.885 | -18.340 | -0.455 |
| FeSO4+ | 4.709e-021 | 4.103e-021 | -20.327 | -20.387 | -0.060 |
| Fe(SO4)2- | 1.576e-023 | 1.373e-023 | -22.803 | -22.862 | -0.060 |
| Fe2(OH)2+4 | 1.306e-026 | 1.590e-027 | -25.884 | -26.799 | -0.915 |
| Fe3(OH)4+5 | 5.573e-035 | 2.200e-036 | -34.254 | -35.658 | -1.404 |
| H(0) | 0.000e+000 | | | | |
| H2 | 0.000e+000 | 0.000e+000 | -46.307 | -46.305 | 0.002 |
| Li | 1.002e-013 | | | | |
| Li+ | 1.001e-013 | 8.811e-014 | -13.000 | -13.055 | -0.055 |
| LiSO4- | 8.066e-017 | 7.029e-017 | -16.093 | -16.153 | -0.060 |
| LiOH | 5.253e-021 | 5.253e-021 | -20.280 | -20.280 | 0.000 |
| Mg | 2.755e-008 | | | | |
| Mg+2 | 2.497e-008 | 1.545e-008 | -7.603 | -7.811 | -0.209 |
| MgHCO3+ | 2.128e-009 | 1.855e-009 | -8.672 | -8.732 | -0.060 |
| MgSO4 | 4.293e-010 | 4.293e-010 | -9.367 | -9.367 | 0.000 |
| MgCO3 | 1.403e-011 | 1.403e-011 | -10.853 | -10.853 | 0.000 |
| Mg4(OH)4+4 | 0.000e+000 | 0.000e+000 | -44.418 | -45.333 | -0.915 |
| Na | 1.302e-003 | | | | |
| Na+ | 1.281e-003 | 1.116e-003 | -2.893 | -2.952 | -0.060 |
| NaHCO3 | 2.043e-005 | 2.043e-005 | -4.690 | -4.690 | 0.000 |
| NaSO4- | 1.146e-006 | 9.989e-007 | -5.941 | -6.000 | -0.060 |
| NaCO3- | 5.741e-009 | 5.003e-009 | -8.241 | -8.301 | -0.060 |
| NaHSiO3 | 1.489e-010 | 1.489e-010 | -9.827 | -9.827 | 0.000 |
| NaAlO2 | 1.603e-011 | 1.603e-011 | -10.795 | -10.795 | 0.000 |
| NaOH | 2.260e-012 | 2.260e-012 | -11.646 | -11.646 | 0.000 |
| O(0) | 2.343e-003 | | | | |
| O2 | 1.172e-003 | 1.177e-003 | -2.931 | -2.929 | 0.002 |
| S(-2) | 0.000e+000 | | | | |
| H2S | 0.000e+000 | 0.000e+000 | -147.240 | -147.240 | 0.000 |
| HS- | 0.000e+000 | 0.000e+000 | -147.914 | -147.975 | -0.061 |
| S-2 | 0.000e+000 | 0.000e+000 | -154.554 | -154.787 | -0.232 |
| S2-2 | 0.000e+000 | 0.000e+000 | -262.597 | -262.838 | -0.242 |
| S3-2 | 0.000e+000 | 0.000e+000 | -370.685 | -370.927 | -0.242 |

```
  S4-2              0.000e+000  0.000e+000  -479.005  -479.247    -0.242
  S5-2              0.000e+000  0.000e+000  -587.551  -587.793    -0.242
S(2)          0.000e+000
  S2O3-2            0.000e+000  0.000e+000  -153.139  -153.381    -0.242
  HS2O3-            0.000e+000  0.000e+000  -158.723  -158.782    -0.060
S(3)          0.000e+000
  S2O4-2            0.000e+000  0.000e+000  -138.854  -139.087    -0.232
S(4)          0.000e+000
  HSO3-             0.000e+000  0.000e+000   -49.827   -49.887    -0.060
  SO3-2             0.000e+000  0.000e+000   -50.413   -50.650    -0.237
  H2SO3             0.000e+000  0.000e+000   -54.268   -54.268     0.000
  SO2               0.000e+000  0.000e+000   -54.521   -54.521     0.000
  S2O6-2            0.000e+000  0.000e+000   -72.395   -72.636    -0.242
  S3O6-2            0.000e+000  0.000e+000  -183.013  -183.254    -0.242
  S4O6-2            0.000e+000  0.000e+000  -277.365  -277.607    -0.242
  S5O6-2            0.000e+000  0.000e+000  -401.223  -401.464    -0.242
S(5)          0.000e+000
  S2O5-2            0.000e+000  0.000e+000  -104.341  -104.583    -0.242
S(6)          3.005e-004
  SO4-2             2.363e-004  1.355e-004    -3.627    -3.868    -0.242
  CaSO4             6.307e-005  6.307e-005    -4.200    -4.200     0.000
  NaSO4-            1.146e-006  9.989e-007    -5.941    -6.000    -0.060
  HSO4-             4.553e-009  3.967e-009    -8.342    -8.402    -0.060
  MgSO4             4.293e-010  4.293e-010    -9.367    -9.367     0.000
  AlSO4+            2.893e-010  2.521e-010    -9.539    -9.598    -0.060
  Al(SO4)2-         3.042e-012  2.651e-012   -11.517   -11.577    -0.060
  LiSO4-            8.066e-017  7.029e-017   -16.093   -16.153    -0.060
  H2SO4             1.904e-018  1.904e-018   -17.720   -17.720     0.000
  FeSO4+            4.709e-021  4.103e-021   -20.327   -20.387    -0.060
  FeSO4             1.176e-022  1.176e-022   -21.930   -21.930     0.000
  Fe(SO4)2-         1.576e-023  1.373e-023   -22.803   -22.862    -0.060
S(7)          0.000e+000
  S2O8-2            0.000e+000  0.000e+000   -45.428   -45.670    -0.242
S(8)          1.590e-030
  HSO5-             1.590e-030  1.386e-030   -29.799   -29.858    -0.060
Si            1.109e-005
  SiO2              1.109e-005  1.109e-005    -4.955    -4.955     0.000
  HSiO3-            2.674e-009  2.330e-009    -8.573    -8.633    -0.060
  NaHSiO3           1.489e-010  1.489e-010    -9.827    -9.827     0.000
  H2SiO4-2          1.436e-015  8.235e-016   -14.843   -15.084    -0.242
  H6(H2SiO4)4-2     4.078e-021  2.338e-021   -20.390   -20.631    -0.242
  H4(H2SiO4)4-4     7.395e-030  7.946e-031   -29.131   -30.100    -0.969
```

## File 17. Mature Cement, Maximum Ion Content, Cement Rebar, Carbon Steel

*INPUT FILE*

```
SOLUTION 1
    temp      15
    pH        7.5
    pe        4
    redox     pe
    units     mmol/kgw
    density   1
    Alkalinity 0
    Cl(-1)    7.5
    Li        1e-010
    Al        1e-010
    Ca        3.1
    Mg        5
    Na        18
    K         1.9
```

```
    S(6)      7.3
    N(5)      7.9
    C(4)      21.8
    Br(-1)    0
    Si        0.01
    -water    1 # kg

GAS_PHASE 1
    -fixed_pressure
    -pressure 1
    -volume 1000
    -temperature 25
    CO2(g)    0.056
    O2(g)     0.18
EQUILIBRIUM_PHASES 1
    Brucite   0 1.39
    Ca(OH)2*(CSH(1.5)) 0 9.5
    Calcite   0 0.001
    CSH(1.0-2.5) 0 15.96
    Gibbsite  0 0.001
    goethite  0 1e-005
    SiO2(am)  0 0.02
REACTION 1
    Fe        1
    4.75 moles in 60 steps
SAVE solution 1-1
END
USE solution 1
GAS_PHASE 2
    -fixed_pressure
    -pressure 1
    -volume 1000
    -temperature 25
    CO2(g)    0.056
    O2(g)     0.18
EQUILIBRIUM_PHASES 2
    calcite   0 1e-010
    Fe(OH)3   0 1e-010
    goethite  0 1e-010
    portlandite 0 1e-010
    SiO2(am)  0 1e-010
REACTION 3
    Fe        1
    4.05 moles in 60 steps
```

## *SAMPLE OUTPUT, FINAL TIME STEP (FILE 17)*

```
Reaction step 60.

Using solution 1.       Solution after simulation 1.
Using pure phase assemblage 2.
Using gas phase 2.
Using reaction 3.

Reaction 3.       Irreversible reaction defined in simulation 2.

        4.050e+000 moles of the following reaction have been added:

                    Relative
        Reactant          moles

        Fe                1.00000
```

| Element | Relative moles |
|---|---|
| Fe | 1.00000 |

----------Gas phase----------

Total pressure: 1.0000 atmospheres
Gas volume: 1.55e+002 liters

| Component | log P | P | Moles in gas: Initial | Final | Delta |
|---|---|---|---|---|---|
| CO2(g) | -0.46 | 3.430e-001 | 2.289e+000 | 2.256e+000 | -3.314e-002 |
| O2(g) | -0.18 | 6.570e-001 | 7.357e+000 | 4.320e+000 | -3.037e+000 |

----------Phase assemblage----------

| Phase | SI log IAP | log KT | Moles in assemblage: Initial | Final | Delta |
|---|---|---|---|---|---|
| Calcite | -0.02 | 1.96 | 1.98 | 1.000e-010 | 0 -1.000e-010 |
| Fe(OH)3 | -5.25 | 0.91 | 6.15 | 1.000e-010 | 0 -1.000e-010 |
| Goethite | -0.00 | 0.91 | 0.91 | 1.000e-010 | 4.050e+000 4.050e+000 |
| Portlandite | -13.14 | 10.19 | 23.33 | 1.000e-010 | 0 -1.000e-010 |
| SiO2(am) | -1.75 | -4.63 | -2.87 | 1.000e-010 | 0 -1.000e-010 |

----------Solution composition----------

| Elements | Molality | Moles |
|---|---|---|
| Al | 8.758e-004 | 8.429e-004 |
| C | 3.444e-002 | 3.315e-002 |
| Ca | 6.867e-003 | 6.608e-003 |
| Cl | 7.793e-003 | 7.500e-003 |
| Fe | 1.659e-011 | 1.597e-011 |
| K | 1.974e-003 | 1.900e-003 |
| Li | 1.039e-013 | 1.000e-013 |
| Mg | 2.814e-008 | 2.708e-008 |
| N | 8.209e-003 | 7.900e-003 |
| Na | 1.870e-002 | 1.800e-002 |
| S | 7.585e-003 | 7.300e-003 |
| Si | 2.359e-005 | 2.270e-005 |

----------Description of solution----------

pH = 6.394 Charge balance
pe = 15.088 Adjusted to redox equilibrium
Activity of water = 0.999
Ionic strength = 5.206e-002
Mass of water (kg) = 9.624e-001
Total alkalinity (eq/kg) = 2.091e-002
Total CO2 (mol/kg) = 3.444e-002
Temperature (deg C) = 15.000
Electrical balance (eq) = -1.448e-002
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -19.24
Iterations = 28
Total H = 1.068919e+002
Total O = 5.357717e+001

----------Distribution of species----------

| Species | Molality | Log Activity | Log Molality | Log Activity | Gamma |
|---|---|---|---|---|---|
| H+ | 4.710e-007 | 4.039e-007 | -6.327 | -6.394 | -0.067 |
| OH- | 1.336e-008 | 1.088e-008 | -7.874 | -7.963 | -0.089 |
| H2O | 5.553e+001 | 9.986e-001 | 1.744 | -0.001 | 0.000 |
| Al | 8.758e-004 | | | | |
| Al13O4(OH)24+7 | 6.734e-005 | 8.637e-009 | -4.172 | -8.064 | -3.892 |
| HAlO2 | 1.314e-007 | 1.314e-007 | -6.881 | -6.881 | 0.000 |
| Al(OH)2+ | 8.505e-008 | 6.968e-008 | -7.070 | -7.157 | -0.087 |
| AlO2- | 8.150e-008 | 6.677e-008 | -7.089 | -7.175 | -0.087 |
| AlOH+2 | 5.275e-008 | 2.398e-008 | -7.278 | -7.620 | -0.342 |
| Al+3 | 7.154e-009 | 1.727e-009 | -8.145 | -8.763 | -0.617 |
| AlSO4+ | 6.004e-009 | 4.919e-009 | -8.222 | -8.308 | -0.087 |
| Al(SO4)2- | 1.297e-009 | 1.063e-009 | -8.887 | -8.973 | -0.087 |
| NaAlO2 | 1.639e-010 | 1.639e-010 | -9.785 | -9.785 | 0.000 |
| Al2(OH)2+4 | 7.476e-012 | 3.720e-013 | -11.126 | -12.429 | -1.303 |
| Al3(OH)4+5 | 2.447e-013 | 2.535e-015 | -12.611 | -14.596 | -1.985 |
| C(-2) | 0.000e+000 | | | | |
| C2H4 | 0.000e+000 | 0.000e+000 | -271.117 | -271.117 | 0.000 |
| C(-3) | 0.000e+000 | | | | |
| C2H6 | 0.000e+000 | 0.000e+000 | -242.876 | -242.876 | 0.000 |
| C(-4) | 0.000e+000 | | | | |
| CH4 | 0.000e+000 | 0.000e+000 | -151.571 | -151.571 | 0.000 |
| C(2) | 0.000e+000 | | | | |
| CO | 0.000e+000 | 0.000e+000 | -50.077 | -50.077 | 0.000 |
| C(4) | 3.444e-002 | | | | |
| HCO3- | 1.783e-002 | 1.461e-002 | -1.749 | -1.835 | -0.087 |
| CO2 | 1.570e-002 | 1.590e-002 | -1.804 | -1.799 | 0.005 |
| CaHCO3+ | 5.312e-004 | 4.352e-004 | -3.275 | -3.361 | -0.087 |
| NaHCO3 | 3.728e-004 | 3.728e-004 | -3.429 | -3.429 | 0.000 |
| CaCO3 | 6.068e-006 | 6.068e-006 | -5.217 | -5.217 | 0.000 |
| CO3-2 | 2.862e-006 | 1.301e-006 | -5.543 | -5.886 | -0.342 |
| NaCO3- | 1.059e-007 | 8.679e-008 | -6.975 | -7.062 | -0.087 |
| MgHCO3+ | 2.100e-009 | 1.721e-009 | -8.678 | -8.764 | -0.087 |
| MgCO3 | 1.237e-011 | 1.237e-011 | -10.907 | -10.907 | 0.000 |
| FeCO3+ | 1.225e-014 | 1.004e-014 | -13.912 | -13.998 | -0.087 |
| FeHCO3+ | 5.896e-020 | 4.831e-020 | -19.229 | -19.316 | -0.087 |
| FeCO3 | 5.741e-022 | 5.741e-022 | -21.241 | -21.241 | 0.000 |
| Ca | 6.867e-003 | | | | |
| Ca+2 | 5.276e-003 | 2.550e-003 | -2.278 | -2.593 | -0.316 |
| CaSO4 | 9.468e-004 | 9.468e-004 | -3.024 | -3.024 | 0.000 |
| CaHCO3+ | 5.312e-004 | 4.352e-004 | -3.275 | -3.361 | -0.087 |
| CaNO3+ | 1.023e-004 | 8.383e-005 | -3.990 | -4.077 | -0.087 |
| CaCO3 | 6.068e-006 | 6.068e-006 | -5.217 | -5.217 | 0.000 |
| CaCl+ | 4.044e-006 | 3.313e-006 | -5.393 | -5.480 | -0.087 |
| CaCl2 | 2.732e-008 | 2.732e-008 | -7.563 | -7.563 | 0.000 |
| CaOH+ | 1.087e-009 | 8.905e-010 | -8.964 | -9.050 | -0.087 |
| Cl(-1) | 7.793e-003 | | | | |
| Cl- | 7.774e-003 | 6.290e-003 | -2.109 | -2.201 | -0.092 |
| NaCl | 1.510e-005 | 1.510e-005 | -4.821 | -4.821 | 0.000 |
| CaCl+ | 4.044e-006 | 3.313e-006 | -5.393 | -5.480 | -0.087 |
| KCl | 2.685e-007 | 2.685e-007 | -6.571 | -6.571 | 0.000 |
| CaCl2 | 2.732e-008 | 2.732e-008 | -7.563 | -7.563 | 0.000 |
| HCl | 5.599e-010 | 5.599e-010 | -9.252 | -9.252 | 0.000 |
| MgCl+ | 6.312e-011 | 5.172e-011 | -10.200 | -10.286 | -0.087 |
| LiCl | 1.643e-017 | 1.643e-017 | -16.784 | -16.784 | 0.000 |
| FeCl2+ | 3.472e-021 | 2.845e-021 | -20.459 | -20.546 | -0.087 |
| FeCl+2 | 7.356e-022 | 3.343e-022 | -21.133 | -21.476 | -0.342 |
| FeCl+ | 3.387e-023 | 2.775e-023 | -22.470 | -22.557 | -0.087 |

| | | | | | |
|---|---|---|---|---|---|
| FeCl2 | 8.903e-028 | 8.903e-028 | -27.050 | -27.050 | 0.000 |
| FeCl4- | 1.652e-028 | 1.353e-028 | -27.782 | -27.869 | -0.087 |
| FeCl4-2 | 2.261e-031 | 1.004e-031 | -30.646 | -30.998 | -0.352 |
| Cl(1) | 9.929e-019 | | | | |
| HClO | 9.181e-019 | 9.181e-019 | -18.037 | -18.037 | 0.000 |
| ClO- | 7.481e-020 | 6.129e-020 | -19.126 | -19.213 | -0.087 |
| Cl(3) | 1.210e-029 | | | | |
| ClO2- | 1.209e-029 | 9.907e-030 | -28.917 | -29.004 | -0.087 |
| HClO2 | 5.916e-033 | 5.916e-033 | -32.228 | -32.228 | 0.000 |
| Cl(5) | 4.210e-025 | | | | |
| ClO3- | 4.210e-025 | 3.428e-025 | -24.376 | -24.465 | -0.089 |
| Cl(7) | 6.109e-025 | | | | |
| ClO4- | 6.109e-025 | 4.975e-025 | -24.214 | -24.303 | -0.089 |
| Fe(2) | 7.539e-020 | | | | |
| FeHCO3+ | 5.896e-020 | 4.831e-020 | -19.229 | -19.316 | -0.087 |
| Fe+2 | 1.304e-020 | 6.300e-021 | -19.885 | -20.201 | -0.316 |
| FeSO4 | 2.780e-021 | 2.780e-021 | -20.556 | -20.556 | 0.000 |
| FeCO3 | 5.741e-022 | 5.741e-022 | -21.241 | -21.241 | 0.000 |
| FeCl+ | 3.387e-023 | 2.775e-023 | -22.470 | -22.557 | -0.087 |
| FeOH+ | 6.012e-024 | 4.926e-024 | -23.221 | -23.308 | -0.087 |
| FeCl2 | 8.903e-028 | 8.903e-028 | -27.050 | -27.050 | 0.000 |
| Fe(OH)2 | 9.674e-029 | 9.674e-029 | -28.014 | -28.014 | 0.000 |
| FeCl4-2 | 2.261e-031 | 1.004e-031 | -30.646 | -30.998 | -0.352 |
| Fe(OH)3- | 1.162e-032 | 9.521e-033 | -31.935 | -32.021 | -0.087 |
| Fe(OH)4-2 | 0.000e+000 | 0.000e+000 | -40.276 | -40.628 | -0.352 |
| Fe(3) | 1.659e-011 | | | | |
| Fe(OH)2+ | 8.502e-012 | 6.966e-012 | -11.070 | -11.157 | -0.087 |
| Fe(OH)3 | 8.055e-012 | 8.055e-012 | -11.094 | -11.094 | 0.000 |
| FeOH+2 | 1.872e-014 | 8.509e-015 | -13.728 | -14.070 | -0.342 |
| FeCO3+ | 1.225e-014 | 1.004e-014 | -13.912 | -13.998 | -0.087 |
| Fe(OH)4- | 6.106e-015 | 5.002e-015 | -14.214 | -14.301 | -0.087 |
| Fe+3 | 2.208e-018 | 5.330e-019 | -17.656 | -18.273 | -0.617 |
| FeSO4+ | 1.199e-019 | 9.826e-020 | -18.921 | -19.008 | -0.087 |
| FeNO3+2 | 7.693e-020 | 3.496e-020 | -19.114 | -19.456 | -0.342 |
| Fe(SO4)2- | 8.247e-021 | 6.757e-021 | -20.084 | -20.170 | -0.087 |
| FeCl2+ | 3.472e-021 | 2.845e-021 | -20.459 | -20.546 | -0.087 |
| FeCl+2 | 7.356e-022 | 3.343e-022 | -21.133 | -21.476 | -0.342 |
| Fe2(OH)2+4 | 3.916e-026 | 1.949e-027 | -25.407 | -26.710 | -1.303 |
| FeCl4- | 1.652e-028 | 1.353e-028 | -27.782 | -27.869 | -0.087 |
| FeNO2+2 | 5.240e-032 | 2.382e-032 | -31.281 | -31.623 | -0.342 |
| Fe3(OH)4+5 | 2.737e-034 | 2.836e-036 | -33.563 | -35.547 | -1.985 |
| H(0) | 0.000e+000 | | | | |
| H2 | 0.000e+000 | 0.000e+000 | -46.278 | -46.272 | 0.005 |
| K | 1.974e-003 | | | | |
| K+ | 1.933e-003 | 1.564e-003 | -2.714 | -2.806 | -0.092 |
| KSO4- | 4.115e-005 | 3.371e-005 | -4.386 | -4.472 | -0.087 |
| KCl | 2.685e-007 | 2.685e-007 | -6.571 | -6.571 | 0.000 |
| KOH | 1.341e-011 | 1.341e-011 | -10.873 | -10.873 | 0.000 |
| KHSO4 | 8.272e-012 | 8.272e-012 | -11.082 | -11.082 | 0.000 |
| Li | 1.039e-013 | | | | |
| Li+ | 1.022e-013 | 8.550e-014 | -12.991 | -13.068 | -0.077 |
| LiSO4- | 1.711e-015 | 1.402e-015 | -14.767 | -14.853 | -0.087 |
| LiCl | 1.643e-017 | 1.643e-017 | -16.784 | -16.784 | 0.000 |
| LiOH | 4.843e-021 | 4.843e-021 | -20.315 | -20.315 | 0.000 |
| Mg | 2.814e-008 | | | | |
| Mg+2 | 2.004e-008 | 1.037e-008 | -7.698 | -7.984 | -0.286 |
| MgSO4 | 5.923e-009 | 5.923e-009 | -8.227 | -8.227 | 0.000 |
| MgHCO3+ | 2.100e-009 | 1.721e-009 | -8.678 | -8.764 | -0.087 |
| MgCl+ | 6.312e-011 | 5.172e-011 | -10.200 | -10.286 | -0.087 |
| MgCO3 | 1.237e-011 | 1.237e-011 | -10.907 | -10.907 | 0.000 |
| Mg4(OH)4+4 | 0.000e+000 | 0.000e+000 | -44.811 | -46.114 | -1.303 |
| N(-03) | 0.000e+000 | | | | |

| | | | | | |
|---|---|---|---|---|---|
| N3- | 0.000e+000 | 0.000e+000 | -99.926 | -100.013 | -0.087 |
| HN3 | 0.000e+000 | 0.000e+000 | -101.612 | -101.612 | 0.000 |
| N(-3) | 0.000e+000 | | | | |
| NH4+ | 0.000e+000 | 0.000e+000 | -63.743 | -63.838 | -0.095 |
| NH3 | 0.000e+000 | 0.000e+000 | -66.999 | -66.999 | 0.000 |
| NH4SO4- | 0.000e+000 | 0.000e+000 | -74.921 | -75.008 | -0.087 |
| N(0) | 2.789e-018 | | | | |
| N2 | 1.395e-018 | 1.395e-018 | -17.856 | -17.856 | 0.000 |
| N(3) | 3.912e-017 | | | | |
| NO2- | 3.909e-017 | 3.163e-017 | -16.408 | -16.500 | -0.092 |
| HNO2 | 2.701e-020 | 2.701e-020 | -19.568 | -19.568 | 0.000 |
| FeNO2+2 | 5.240e-032 | 2.382e-032 | -31.281 | -31.623 | -0.342 |
| N(5) | 8.209e-003 | | | | |
| NO3- | 8.107e-003 | 6.560e-003 | -2.091 | -2.183 | -0.092 |
| CaNO3+ | 1.023e-004 | 8.383e-005 | -3.990 | -4.077 | -0.087 |
| HNO3 | 1.090e-010 | 1.090e-010 | -9.963 | -9.963 | 0.000 |
| FeNO3+2 | 7.693e-020 | 3.496e-020 | -19.114 | -19.456 | -0.342 |
| Na | 1.870e-002 | | | | |
| Na+ | 1.798e-002 | 1.474e-002 | -1.745 | -1.832 | -0.087 |
| NaHCO3 | 3.728e-004 | 3.728e-004 | -3.429 | -3.429 | 0.000 |
| NaSO4- | 3.308e-004 | 2.710e-004 | -3.480 | -3.567 | -0.087 |
| NaCl | 1.510e-005 | 1.510e-005 | -4.821 | -4.821 | 0.000 |
| NaCO3- | 1.059e-007 | 8.679e-008 | -6.975 | -7.062 | -0.087 |
| NaHSiO3 | 3.970e-009 | 3.970e-009 | -8.401 | -8.401 | 0.000 |
| NaAlO2 | 1.639e-010 | 1.639e-010 | -9.785 | -9.785 | 0.000 |
| NaOH | 2.834e-011 | 2.834e-011 | -10.548 | -10.548 | 0.000 |
| O(0) | 1.999e-003 | | | | |
| O2 | 9.995e-004 | 1.012e-003 | -3.000 | -2.995 | 0.005 |
| S(-2) | 0.000e+000 | | | | |
| H2S | 0.000e+000 | 0.000e+000 | -145.752 | -145.752 | 0.000 |
| HS- | 0.000e+000 | 0.000e+000 | -146.420 | -146.509 | -0.089 |
| S-2 | 0.000e+000 | 0.000e+000 | -153.009 | -153.343 | -0.333 |
| S2-2 | 0.000e+000 | 0.000e+000 | -259.586 | -259.939 | -0.352 |
| S3-2 | 0.000e+000 | 0.000e+000 | -366.220 | -366.572 | -0.352 |
| S4-2 | 0.000e+000 | 0.000e+000 | -473.084 | -473.436 | -0.352 |
| S5-2 | 0.000e+000 | 0.000e+000 | -580.174 | -580.527 | -0.352 |
| S(2) | 0.000e+000 | | | | |
| S2O3-2 | 0.000e+000 | 0.000e+000 | -150.227 | -150.579 | -0.352 |
| HS2O3- | 0.000e+000 | 0.000e+000 | -155.873 | -155.959 | -0.087 |
| S(3) | 0.000e+000 | | | | |
| S2O4-2 | 0.000e+000 | 0.000e+000 | -135.985 | -136.318 | -0.333 |
| S(4) | 0.000e+000 | | | | |
| HSO3- | 0.000e+000 | 0.000e+000 | -48.433 | -48.519 | -0.087 |
| SO3-2 | 0.000e+000 | 0.000e+000 | -48.962 | -49.304 | -0.342 |
| H2SO3 | 0.000e+000 | 0.000e+000 | -52.878 | -52.878 | 0.000 |
| SO2 | 0.000e+000 | 0.000e+000 | -53.131 | -53.131 | 0.000 |
| S2O6-2 | 0.000e+000 | 0.000e+000 | -69.581 | -69.934 | -0.352 |
| S3O6-2 | 0.000e+000 | 0.000e+000 | -178.744 | -179.096 | -0.352 |
| S4O6-2 | 0.000e+000 | 0.000e+000 | -271.641 | -271.993 | -0.352 |
| S5O6-2 | 0.000e+000 | 0.000e+000 | -394.043 | -394.395 | -0.352 |
| S(5) | 0.000e+000 | | | | |
| S2O5-2 | 0.000e+000 | 0.000e+000 | -101.495 | -101.848 | -0.352 |
| S(6) | 7.585e-003 | | | | |
| SO4-2 | 6.267e-003 | 2.784e-003 | -2.203 | -2.555 | -0.352 |
| CaSO4 | 9.468e-004 | 9.468e-004 | -3.024 | -3.024 | 0.000 |
| NaSO4- | 3.308e-004 | 2.710e-004 | -3.480 | -3.567 | -0.087 |
| KSO4- | 4.115e-005 | 3.371e-005 | -4.386 | -4.472 | -0.087 |
| HSO4- | 1.046e-007 | 8.574e-008 | -6.980 | -7.067 | -0.087 |
| AlSO4+ | 6.004e-009 | 4.919e-009 | -8.222 | -8.308 | -0.087 |
| MgSO4 | 5.923e-009 | 5.923e-009 | -8.227 | -8.227 | 0.000 |
| Al(SO4)2- | 1.297e-009 | 1.063e-009 | -8.887 | -8.973 | -0.087 |
| KHSO4 | 8.272e-012 | 8.272e-012 | -11.082 | -11.082 | 0.000 |

```
   LiSO4-              1.711e-015  1.402e-015   -14.767   -14.853    -0.087
   H2SO4               4.328e-017  4.328e-017   -16.364   -16.364     0.000
   FeSO4+              1.199e-019  9.826e-020   -18.921   -19.008    -0.087
   Fe(SO4)2-           8.247e-021  6.757e-021   -20.084   -20.170    -0.087
   FeSO4               2.780e-021  2.780e-021   -20.556   -20.556     0.000
   NH4SO4-             0.000e+000  0.000e+000   -74.921   -75.008    -0.087
S(7)          0.000e+000
   S2O8-2              0.000e+000  0.000e+000   -42.680   -43.033    -0.352
S(8)          3.389e-029
   HSO5-               3.389e-029  2.777e-029   -28.470   -28.556    -0.087
Si            2.359e-005
   SiO2                2.358e-005  2.358e-005    -4.628    -4.628     0.000
   HSiO3-              5.743e-009  4.706e-009    -8.241    -8.327    -0.087
   NaHSiO3             3.970e-009  3.970e-009    -8.401    -8.401     0.000
   H2SiO4-2            3.557e-015  1.580e-015   -14.449   -14.801    -0.352
   H6(H2SiO4)4-2       9.656e-020  4.290e-020   -19.015   -19.368    -0.352
   H4(H2SiO4)4-4       3.433e-028  1.318e-029   -27.464   -28.880    -1.416
```

## File 18. Mature Cement, Maximum Ion Content, Cement Rebar, Stainless Steel

*INPUT FILE*

```
SOLUTION 1
   temp      15
   pH        7.5
   pe        4
   redox     pe
   units     mmol/kgw
   density   1
   Alkalinity 0
   Cl(-1)    7.5
   Li        1e-010
   Al        1e-010
   Ca        3.1
   Mg        5
   Na        18
   K         1.9
   S(6)      7.3
   N(5)      7.9
   C(4)      21.8
   Br(-1)    0
   Si        0.01
   -water    1 # kg

GAS_PHASE 1
   -fixed_pressure
   -pressure 1
   -volume 1000
   -temperature 25
   CO2(g)    0.056
   O2(g)     0.18
EQUILIBRIUM_PHASES 1
   Brucite   0 1.39
   Ca(OH)2*(CSH(1.5)) 0 9.5
   Calcite   0 0.001
   CSH(1.0-2.5) 0 15.96
   Gibbsite  0 0.001
   goethite  0 1e-005
   SiO2(am)  0 0.02
REACTION 1
   Fe        1
   4.75 moles in 60 steps
```

```
SAVE solution 1-1
END
USE solution 1
GAS_PHASE 2
   -fixed_pressure
   -pressure 1
   -volume 1000
   -temperature 25
   CO2(g)    0.056
   O2(g)     0.18
EQUILIBRIUM_PHASES 2
   calcite   0 1e-010
   Fe(OH)3   0 1e-010
   goethite  0 1e-010
   portlandite 0 1e-010
   SiO2(am)  0 1e-010
REACTION 3
   Fe        1
   0.025 moles in 60 steps
```

## *SAMPLE OUTPUT, FINAL TIME STEP (FILE 18)*

```
Reaction step 60.

Using solution 1.       Solution after simulation 1.
Using pure phase assemblage 2.
Using gas phase 2.
Using reaction 3.

Reaction 3.       Irreversible reaction defined in simulation 2.

      2.500e-002 moles of the following reaction have been added:

                  Relative
      Reactant          moles

      Fe                1.00000

                  Relative
      Element           moles
      Fe                1.00000

-----------------------------------Gas phase-----------------------------------


Total pressure:   1.0000   atmospheres
   Gas volume:  2.27e+002 liters

                                          Moles in gas
                                  ----------------------------------
Component             log P          P     Initial       Final       Delta

CO2(g)                -0.63  2.355e-001  2.289e+000  2.261e+000 -2.813e-002
O2(g)                 -0.12  7.645e-001  7.357e+000  7.339e+000 -1.839e-002

--------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
Phase               SI log IAP  log KT      Initial       Final       Delta

Calcite           -0.00    1.98    1.98   1.000e-010  6.734e-004  6.734e-004
Fe(OH)3           -5.25    0.91    6.15   1.000e-010           0 -1.000e-010
```

| | | | | | | |
|---|---|---|---|---|---|---|
| Goethite | -0.00 | 0.91 | 0.91 | 1.000e-010 | 2.500e-002 | 2.500e-002 |
| Portlandite | -12.96 | 10.37 | 23.33 | 1.000e-010 | 0 | -1.000e-010 |
| SiO2(am) | -1.77 | -4.64 | -2.87 | 1.000e-010 | 0 | -1.000e-010 |

----------Solution composition----------

| Elements | Molality | Moles |
|---|---|---|
| Al | 8.440e-004 | 8.429e-004 |
| C | 2.750e-002 | 2.746e-002 |
| Ca | 5.943e-003 | 5.935e-003 |
| Cl | 7.510e-003 | 7.500e-003 |
| Fe | 1.454e-011 | 1.452e-011 |
| K | 1.903e-003 | 1.900e-003 |
| Li | 1.001e-013 | 1.000e-013 |
| Mg | 2.712e-008 | 2.708e-008 |
| N | 7.911e-003 | 7.900e-003 |
| Na | 1.802e-002 | 1.800e-002 |
| S | 7.310e-003 | 7.300e-003 |
| Si | 2.273e-005 | 2.270e-005 |

----------Description of solution----------

pH = 6.511 Charge balance
pe = 14.987 Adjusted to redox equilibrium
Activity of water = 0.999
Ionic strength = 4.870e-002
Mass of water (kg) = 9.986e-001
Total alkalinity (eq/kg) = 1.880e-002
Total CO2 (mol/kg) = 2.750e-002
Temperature (deg C) = 15.000
Electrical balance (eq) = -1.448e-002
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -19.79
Iterations = 35
Total H = 1.109169e+002
Total O = 5.557803e+001

----------Distribution of species----------

| Species | Molality | Log Activity | Log Molality | Log Activity | Gamma |
|---|---|---|---|---|---|
| H+ | 3.586e-007 | 3.084e-007 | -6.445 | -6.511 | -0.066 |
| OH- | 1.741e-008 | 1.425e-008 | -7.759 | -7.846 | -0.087 |
| H2O | 5.553e+001 | 9.987e-001 | 1.744 | -0.001 | 0.000 |
| Al | 8.440e-004 | | | | |
| Al13O4(OH)24+7 | 6.490e-005 | 1.022e-008 | -4.188 | -7.991 | -3.803 |
| HAlO2 | 1.539e-007 | 1.539e-007 | -6.813 | -6.813 | 0.000 |
| AlO2- | 1.244e-007 | 1.024e-007 | -6.905 | -6.990 | -0.084 |
| Al(OH)2+ | 7.569e-008 | 6.232e-008 | -7.121 | -7.205 | -0.084 |
| AlOH+2 | 3.533e-008 | 1.637e-008 | -7.452 | -7.786 | -0.334 |
| Al+3 | 3.626e-009 | 9.000e-010 | -8.441 | -9.046 | -0.605 |
| AlSO4+ | 3.103e-009 | 2.555e-009 | -8.508 | -8.593 | -0.084 |
| Al(SO4)2- | 6.681e-010 | 5.501e-010 | -9.175 | -9.260 | -0.084 |
| NaAlO2 | 2.441e-010 | 2.441e-010 | -9.612 | -9.612 | 0.000 |
| Al2(OH)2+4 | 3.248e-012 | 1.734e-013 | -11.488 | -12.761 | -1.273 |
| Al3(OH)4+5 | 9.189e-014 | 1.057e-015 | -13.037 | -14.976 | -1.939 |
| C(-2) | 0.000e+000 | | | | |
| C2H4 | 0.000e+000 | 0.000e+000 | -271.641 | -271.641 | 0.000 |
| C(-3) | 0.000e+000 | | | | |
| C2H6 | 0.000e+000 | 0.000e+000 | -243.433 | -243.433 | 0.000 |
| C(-4) | 0.000e+000 | | | | |

| | | | | | |
|---|---|---|---|---|---|
| CH4 | 0.000e+000 | 0.000e+000 | -151.866 | -151.866 | 0.000 |
| C(2) | 0.000e+000 | | | | |
| CO | 0.000e+000 | 0.000e+000 | -50.274 | -50.274 | 0.000 |
| C(4) | 2.750e-002 | | | | |
| HCO3- | 1.596e-002 | 1.314e-002 | -1.797 | -1.881 | -0.084 |
| CO2 | 1.078e-002 | 1.091e-002 | -1.967 | -1.962 | 0.005 |
| CaHCO3+ | 4.205e-004 | 3.462e-004 | -3.376 | -3.461 | -0.084 |
| NaHCO3 | 3.253e-004 | 3.253e-004 | -3.488 | -3.488 | 0.000 |
| CaCO3 | 6.322e-006 | 6.322e-006 | -5.199 | -5.199 | 0.000 |
| CO3-2 | 3.307e-006 | 1.532e-006 | -5.481 | -5.815 | -0.334 |
| NaCO3- | 1.205e-007 | 9.920e-008 | -6.919 | -7.003 | -0.084 |
| MgHCO3+ | 1.845e-009 | 1.519e-009 | -8.734 | -8.818 | -0.084 |
| MgCO3 | 1.431e-011 | 1.431e-011 | -10.844 | -10.844 | 0.000 |
| FeCO3+ | 6.389e-015 | 5.261e-015 | -14.195 | -14.279 | -0.084 |
| FeHCO3+ | 2.961e-020 | 2.438e-020 | -19.529 | -19.613 | -0.084 |
| FeCO3 | 3.794e-022 | 3.794e-022 | -21.421 | -21.421 | 0.000 |
| Ca | 5.943e-003 | | | | |
| Ca+2 | 4.591e-003 | 2.255e-003 | -2.338 | -2.647 | -0.309 |
| CaSO4 | 8.345e-004 | 8.345e-004 | -3.079 | -3.079 | 0.000 |
| CaHCO3+ | 4.205e-004 | 3.462e-004 | -3.376 | -3.461 | -0.084 |
| CaNO3+ | 8.740e-005 | 7.196e-005 | -4.058 | -4.143 | -0.084 |
| CaCO3 | 6.322e-006 | 6.322e-006 | -5.199 | -5.199 | 0.000 |
| CaCl+ | 3.450e-006 | 2.840e-006 | -5.462 | -5.547 | -0.084 |
| CaCl2 | 2.270e-008 | 2.270e-008 | -7.644 | -7.644 | 0.000 |
| CaOH+ | 1.253e-009 | 1.032e-009 | -8.902 | -8.986 | -0.084 |
| Cl(-1) | 7.510e-003 | | | | |
| Cl- | 7.492e-003 | 6.096e-003 | -2.125 | -2.215 | -0.090 |
| NaCl | 1.420e-005 | 1.420e-005 | -4.848 | -4.848 | 0.000 |
| CaCl+ | 3.450e-006 | 2.840e-006 | -5.462 | -5.547 | -0.084 |
| KCl | 2.521e-007 | 2.521e-007 | -6.598 | -6.598 | 0.000 |
| CaCl2 | 2.270e-008 | 2.270e-008 | -7.644 | -7.644 | 0.000 |
| HCl | 4.143e-010 | 4.143e-010 | -9.383 | -9.383 | 0.000 |
| MgCl+ | 5.975e-011 | 4.919e-011 | -10.224 | -10.308 | -0.084 |
| LiCl | 1.541e-017 | 1.541e-017 | -16.812 | -16.812 | 0.000 |
| FeCl2+ | 1.444e-021 | 1.189e-021 | -20.840 | -20.925 | -0.084 |
| FeCl+2 | 3.111e-022 | 1.442e-022 | -21.507 | -21.841 | -0.334 |
| FeCl+ | 1.833e-023 | 1.509e-023 | -22.737 | -22.821 | -0.084 |
| FeCl2 | 4.692e-028 | 4.692e-028 | -27.329 | -27.329 | 0.000 |
| FeCl4- | 6.452e-029 | 5.312e-029 | -28.190 | -28.275 | -0.084 |
| FeCl4-2 | 1.096e-031 | 4.972e-032 | -30.960 | -31.304 | -0.343 |
| Cl(1) | 8.106e-019 | | | | |
| HClO | 7.328e-019 | 7.328e-019 | -18.135 | -18.135 | 0.000 |
| ClO- | 7.783e-020 | 6.408e-020 | -19.109 | -19.193 | -0.084 |
| Cl(3) | 1.358e-029 | | | | |
| ClO2- | 1.357e-029 | 1.117e-029 | -28.867 | -28.952 | -0.084 |
| HClO2 | 5.094e-033 | 5.094e-033 | -32.293 | -32.293 | 0.000 |
| Cl(5) | 5.095e-025 | | | | |
| ClO3- | 5.095e-025 | 4.171e-025 | -24.293 | -24.380 | -0.087 |
| Cl(7) | 7.975e-025 | | | | |
| ClO4- | 7.975e-025 | 6.529e-025 | -24.098 | -24.185 | -0.087 |
| Fe(2) | 3.876e-020 | | | | |
| FeHCO3+ | 2.961e-020 | 2.438e-020 | -19.529 | -19.613 | -0.084 |
| Fe+2 | 7.196e-021 | 3.535e-021 | -20.143 | -20.452 | -0.309 |
| FeSO4 | 1.554e-021 | 1.554e-021 | -20.808 | -20.808 | 0.000 |
| FeCO3 | 3.794e-022 | 3.794e-022 | -21.421 | -21.421 | 0.000 |
| FeCl+ | 1.833e-023 | 1.509e-023 | -22.737 | -22.821 | -0.084 |
| FeOH+ | 4.398e-024 | 3.621e-024 | -23.357 | -23.441 | -0.084 |
| FeCl2 | 4.692e-028 | 4.692e-028 | -27.329 | -27.329 | 0.000 |
| Fe(OH)2 | 9.315e-029 | 9.315e-029 | -28.031 | -28.031 | 0.000 |
| FeCl4-2 | 1.096e-031 | 4.972e-032 | -30.960 | -31.304 | -0.343 |
| Fe(OH)3- | 1.459e-032 | 1.201e-032 | -31.836 | -31.920 | -0.084 |
| Fe(OH)4-2 | 0.000e+000 | 0.000e+000 | -40.067 | -40.410 | -0.343 |

| | | | | | |
|---|---|---|---|---|---|
| Fe(3) | 1.454e-011 | | | | |
| Fe(OH)3 | 8.056e-012 | 8.056e-012 | -11.094 | -11.094 | 0.000 |
| Fe(OH)2+ | 6.460e-012 | 5.318e-012 | -11.190 | -11.274 | -0.084 |
| FeOH+2 | 1.070e-014 | 4.959e-015 | -13.971 | -14.305 | -0.334 |
| Fe(OH)4- | 7.960e-015 | 6.554e-015 | -14.099 | -14.183 | -0.084 |
| FeCO3+ | 6.389e-015 | 5.261e-015 | -14.195 | -14.279 | -0.084 |
| Fe+3 | 9.554e-019 | 2.372e-019 | -18.020 | -18.625 | -0.605 |
| FeSO4+ | 5.291e-020 | 4.357e-020 | -19.276 | -19.361 | -0.084 |
| FeNO3+2 | 3.258e-020 | 1.510e-020 | -19.487 | -19.821 | -0.334 |
| Fe(SO4)2- | 3.625e-021 | 2.985e-021 | -20.441 | -20.525 | -0.084 |
| FeCl2+ | 1.444e-021 | 1.189e-021 | -20.840 | -20.925 | -0.084 |
| FeCl+2 | 3.111e-022 | 1.442e-022 | -21.507 | -21.841 | -0.334 |
| Fe2(OH)2+4 | 1.240e-026 | 6.619e-028 | -25.907 | -27.179 | -1.273 |
| FeCl4- | 6.452e-029 | 5.312e-029 | -28.190 | -28.275 | -0.084 |
| FeNO2+2 | 2.057e-032 | 9.533e-033 | -31.687 | -32.021 | -0.334 |
| Fe3(OH)4+5 | 6.396e-035 | 7.355e-037 | -34.194 | -36.133 | -1.939 |
| H(0) | 0.000e+000 | | | | |
| H2 | 0.000e+000 | 0.000e+000 | -46.310 | -46.305 | 0.005 |
| K | 1.903e-003 | | | | |
| K+ | 1.863e-003 | 1.516e-003 | -2.730 | -2.819 | -0.090 |
| KSO4- | 3.954e-005 | 3.255e-005 | -4.403 | -4.487 | -0.084 |
| KCl | 2.521e-007 | 2.521e-007 | -6.598 | -6.598 | 0.000 |
| KOH | 1.702e-011 | 1.702e-011 | -10.769 | -10.769 | 0.000 |
| KHSO4 | 6.098e-012 | 6.098e-012 | -11.215 | -11.215 | 0.000 |
| Li | 1.001e-013 | | | | |
| Li+ | 9.848e-014 | 8.272e-014 | -13.007 | -13.082 | -0.076 |
| LiSO4- | 1.641e-015 | 1.351e-015 | -14.785 | -14.869 | -0.084 |
| LiCl | 1.541e-017 | 1.541e-017 | -16.812 | -16.812 | 0.000 |
| LiOH | 6.138e-021 | 6.138e-021 | -20.212 | -20.212 | 0.000 |
| Mg | 2.712e-008 | | | | |
| Mg+2 | 1.941e-008 | 1.018e-008 | -7.712 | -7.992 | -0.280 |
| MgSO4 | 5.793e-009 | 5.793e-009 | -8.237 | -8.237 | 0.000 |
| MgHCO3+ | 1.845e-009 | 1.519e-009 | -8.734 | -8.818 | -0.084 |
| MgCl+ | 5.975e-011 | 4.919e-011 | -10.224 | -10.308 | -0.084 |
| MgCO3 | 1.431e-011 | 1.431e-011 | -10.844 | -10.844 | 0.000 |
| Mg4(OH)4+4 | 0.000e+000 | 0.000e+000 | -44.405 | -45.677 | -1.273 |
| N(-03) | 0.000e+000 | | | | |
| N3- | 0.000e+000 | 0.000e+000 | -100.465 | -100.550 | -0.084 |
| HN3 | 0.000e+000 | 0.000e+000 | -102.266 | -102.266 | 0.000 |
| N(-3) | 0.000e+000 | | | | |
| NH4+ | 0.000e+000 | 0.000e+000 | -64.124 | -64.217 | -0.092 |
| NH3 | 0.000e+000 | 0.000e+000 | -67.261 | -67.261 | 0.000 |
| NH4SO4- | 0.000e+000 | 0.000e+000 | -75.304 | -75.388 | -0.084 |
| N(0) | 1.048e-018 | | | | |
| N2 | 5.240e-019 | 5.240e-019 | -18.281 | -18.281 | 0.000 |
| N(3) | 3.499e-017 | | | | |
| NO2- | 3.497e-017 | 2.846e-017 | -16.456 | -16.546 | -0.090 |
| HNO2 | 1.855e-020 | 1.855e-020 | -19.732 | -19.732 | 0.000 |
| FeNO2+2 | 2.057e-032 | 9.533e-033 | -31.687 | -32.021 | -0.334 |
| N(5) | 7.911e-003 | | | | |
| NO3- | 7.823e-003 | 6.366e-003 | -2.107 | -2.196 | -0.090 |
| CaNO3+ | 8.740e-005 | 7.196e-005 | -4.058 | -4.143 | -0.084 |
| HNO3 | 8.075e-011 | 8.075e-011 | -10.093 | -10.093 | 0.000 |
| FeNO3+2 | 3.258e-020 | 1.510e-020 | -19.487 | -19.821 | -0.334 |
| Na | 1.802e-002 | | | | |
| Na+ | 1.737e-002 | 1.430e-002 | -1.760 | -1.845 | -0.084 |
| NaHCO3 | 3.253e-004 | 3.253e-004 | -3.488 | -3.488 | 0.000 |
| NaSO4- | 3.183e-004 | 2.620e-004 | -3.497 | -3.582 | -0.084 |
| NaCl | 1.420e-005 | 1.420e-005 | -4.848 | -4.848 | 0.000 |
| NaCO3- | 1.205e-007 | 9.920e-008 | -6.919 | -7.003 | -0.084 |
| NaHSiO3 | 4.863e-009 | 4.863e-009 | -8.313 | -8.313 | 0.000 |
| NaAlO2 | 2.441e-010 | 2.441e-010 | -9.612 | -9.612 | 0.000 |

| | | | | | |
|---|---|---|---|---|---|
| NaOH | 3.603e-011 | 3.603e-011 | -10.443 | -10.443 | 0.000 |
| O(0) | 2.328e-003 | | | | |
| O2 | 1.164e-003 | 1.178e-003 | -2.934 | -2.929 | 0.005 |
| S(-2) | 0.000e+000 | | | | |
| H2S | 0.000e+000 | 0.000e+000 | -146.120 | -146.120 | 0.000 |
| HS- | 0.000e+000 | 0.000e+000 | -146.673 | -146.760 | -0.087 |
| S-2 | 0.000e+000 | 0.000e+000 | -153.151 | -153.476 | -0.325 |
| S2-2 | 0.000e+000 | 0.000e+000 | -260.063 | -260.407 | -0.343 |
| S3-2 | 0.000e+000 | 0.000e+000 | -367.031 | -367.375 | -0.343 |
| S4-2 | 0.000e+000 | 0.000e+000 | -474.230 | -474.574 | -0.343 |
| S5-2 | 0.000e+000 | 0.000e+000 | -581.655 | -581.999 | -0.343 |
| S(2) | 0.000e+000 | | | | |
| S2O3-2 | 0.000e+000 | 0.000e+000 | -150.605 | -150.949 | -0.343 |
| HS2O3- | 0.000e+000 | 0.000e+000 | -156.361 | -156.446 | -0.084 |
| S(3) | 0.000e+000 | | | | |
| S2O4-2 | 0.000e+000 | 0.000e+000 | -136.329 | -136.655 | -0.325 |
| S(4) | 0.000e+000 | | | | |
| HSO3- | 0.000e+000 | 0.000e+000 | -48.587 | -48.671 | -0.084 |
| SO3-2 | 0.000e+000 | 0.000e+000 | -49.004 | -49.338 | -0.334 |
| H2SO3 | 0.000e+000 | 0.000e+000 | -53.147 | -53.147 | 0.000 |
| SO2 | 0.000e+000 | 0.000e+000 | -53.400 | -53.400 | 0.000 |
| S2O6-2 | 0.000e+000 | 0.000e+000 | -69.861 | -70.204 | -0.343 |
| S3O6-2 | 0.000e+000 | 0.000e+000 | -179.358 | -179.701 | -0.343 |
| S4O6-2 | 0.000e+000 | 0.000e+000 | -272.589 | -272.933 | -0.343 |
| S5O6-2 | 0.000e+000 | 0.000e+000 | -395.327 | -395.670 | -0.343 |
| S(5) | 0.000e+000 | | | | |
| S2O5-2 | 0.000e+000 | 0.000e+000 | -101.808 | -102.151 | -0.343 |
| S(6) | 7.310e-003 | | | | |
| SO4-2 | 6.118e-003 | 2.774e-003 | -2.213 | -2.557 | -0.343 |
| CaSO4 | 8.345e-004 | 8.345e-004 | -3.079 | -3.079 | 0.000 |
| NaSO4- | 3.183e-004 | 2.620e-004 | -3.497 | -3.582 | -0.084 |
| KSO4- | 3.954e-005 | 3.255e-005 | -4.403 | -4.487 | -0.084 |
| HSO4- | 7.922e-008 | 6.523e-008 | -7.101 | -7.186 | -0.084 |
| MgSO4 | 5.793e-009 | 5.793e-009 | -8.237 | -8.237 | 0.000 |
| AlSO4+ | 3.103e-009 | 2.555e-009 | -8.508 | -8.593 | -0.084 |
| Al(SO4)2- | 6.681e-010 | 5.501e-010 | -9.175 | -9.260 | -0.084 |
| KHSO4 | 6.098e-012 | 6.098e-012 | -11.215 | -11.215 | 0.000 |
| LiSO4- | 1.641e-015 | 1.351e-015 | -14.785 | -14.869 | -0.084 |
| H2SO4 | 2.514e-017 | 2.514e-017 | -16.600 | -16.600 | 0.000 |
| FeSO4+ | 5.291e-020 | 4.357e-020 | -19.276 | -19.361 | -0.084 |
| Fe(SO4)2- | 3.625e-021 | 2.985e-021 | -20.441 | -20.525 | -0.084 |
| FeSO4 | 1.554e-021 | 1.554e-021 | -20.808 | -20.808 | 0.000 |
| NH4SO4- | 0.000e+000 | 0.000e+000 | -75.304 | -75.388 | -0.084 |
| S(7) | 0.000e+000 | | | | |
| S2O8-2 | 0.000e+000 | 0.000e+000 | -42.894 | -43.237 | -0.343 |
| S(8) | 2.768e-029 | | | | |
| HSO5- | 2.768e-029 | 2.279e-029 | -28.558 | -28.642 | -0.084 |
| Si | 2.273e-005 | | | | |
| SiO2 | 2.272e-005 | 2.272e-005 | -4.644 | -4.644 | 0.000 |
| HSiO3- | 7.214e-009 | 5.940e-009 | -8.142 | -8.226 | -0.084 |
| NaHSiO3 | 4.863e-009 | 4.863e-009 | -8.313 | -8.313 | 0.000 |
| H2SiO4-2 | 5.762e-015 | 2.613e-015 | -14.239 | -14.583 | -0.343 |
| H6(H2SiO4)4-2 | 1.401e-019 | 6.352e-020 | -18.854 | -19.197 | -0.343 |
| H4(H2SiO4)4-4 | 8.026e-028 | 3.348e-029 | -27.096 | -28.475 | -1.380 |

## A-15. Waste Forms Inside Liners

The solution chemistry inside resin containers was not modeled. The chemistry inside the metal containers was modeled by repeating the calculations previously presented and then adding an additional 0.42 moles of iron per 60-year period. The results were not significantly different from what has already

been summarized, and these modeling results are not provided here. Future investigators should be able to reach the same conclusions by repeating the prior calculations and making the minor modifications as described herein.

## A-15.1 Vault Floor and Sand/Gravel Base

Water that exits the steel waste liners will either penetrate into cracks and pores in the vault floor or flow along cement surfaces. This process is assumed to alter solution chemistry to what it was prior to infiltration of water into the steel liners. Hence, water that exits the vault is assumed to have a general solution composition comparable to that entering the vault. However, once exiting water encounters the sand/gravel underlayment, it will mix with native alluvium water that has not entered the vault. The composition of this exiting solution was modeled using two mixing scenarios for each cement type and groundwater ion composition, yielding a total of 12 input files.

1. Fresh cement (four input files)
   - Minimum ions, Mixture of 95% cement effluent, 5% alluvium water (file 19)
   - Maximum ions, Mixture of 95% cement effluent, 5% alluvium water (file 20)
   - Minimum ions, Mixture of 50% cement effluent, 50% alluvium water (file 21)
   - Maximum ions, Mixture of 50% cement effluent, 50% alluvium water (file 22)
2. Mature cement (four input files)
   - Minimum ions, Mixture of 95% cement effluent, 5% alluvium water (file 23)
   - Maximum ions, Mixture of 95% cement effluent, 5% alluvium water (file 24)
   - Minimum ions, Mixture of 50% cement effluent, 50% alluvium water (file 25)
   - Maximum ions, Mixture of 50% cement effluent, 50% alluvium water (file 26)
3. Degraded cement (four input files)
   - Minimum ions, Mixture of 95% cement effluent, 5% alluvium water (file 27
   - Maximum ions, Mixture of 95% cement effluent, 5% alluvium water (file 28)
   - Minimum ions, Mixture of 50% cement effluent, 50% alluvium water (file 29)
   - Maximum ions, Mixture of 50% cement effluent, 50% alluvium water (file 30)

Input files for these calculations and sample results from them are provided as before. The input file is given first, followed by results from the final time step (or iteration). The same parameters are provided here as were provided previously.

**File 19. Fresh Cement, Minimum ions, 95%/5% Mixing Ratio**

*INPUT FILE*

```
SOLUTION 1
    temp      15
    pH        7.5 charge
    pe        4
    redox     pe
    units     mmol/kgw
    density   1
    Alkalinity 0
    Cl(-1)    0
    Li        1e-010
    Al        1e-010
    Ca        0.6
    Mg        0.3
```

```
    Na        1.3
    K         0
    S(6)      0.3
    N(5)      0
    C(4)      1.4
    Br(-1)    0
    Si        0.01
    -water    0.144 # kg

EQUILIBRIUM_PHASES 1
    Brucite   0 0.208
    Ca(OH)2*(CSH(1.5)) 0 1.42
    Calcite   0 0.001
    CSH(1.0-2.5) 0 2.386
    Ettringite 0 0.016
    Gibbsite  0 0.001
    Goethite  0 0.001
    Hydrogarnet(C3AH6) 0 0.384
    SiO2(am)  0 0.02
    KOH(cement) 0 0.148
    NaOH(cement) 0 0.022
    Monosulfate 0 0.192
GAS_PHASE 1
    -fixed_pressure
    -pressure 1
    -volume 1
    -temperature 25
    CO2(g)    0.056
SAVE solution 1-1
END
SOLUTION 2
    temp      25
    pH        7.5 charge
    pe        4
    redox     pe
    units     mmol/kgs
    density   1
    Li        0
    Alkalinity 0
    Ca        0.6
    Mg        0.3
    Na        1.3
    C(4)      1.4
    Cl        0
    S(6)      0.3
    N(5)      0
    Si        0.001
    K         0
    -water    0.144 # kg
GAS_PHASE 2
    -fixed_pressure
    -pressure 1
    -volume 1
    -temperature 25
    CO2(g)    0.056
    O2(g)     0.18
EQUILIBRIUM_PHASES 2
    calcite   0 1
SAVE solution 2-2
END
MIX 1
    1    0.95
```

```
   2   0.05
EQUILIBRIUM_PHASES 3
   Albite    0 0.6
   Calcite   0 0.1
   K-Feldspar 0 0.6
   Quartz    0 72
   SiO2(am)  0 17.3
```

*SAMPLE OUTPUT, FINAL TIME STEP (FILE 19)*

```
-------------------------------------------
Beginning of batch-reaction calculations.
-------------------------------------------

Reaction step 1.

Using mix 1.
Using pure phase assemblage 3.

Mixture 1.

       9.500e-001 Solution 1       Solution after simulation 1.
       5.000e-002 Solution 2       Solution after simulation 2.

--------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
Phase               SI log IAP  log KT      Initial       Final       Delta

Albite            0.00    2.93    2.93   6.000e-001  4.595e-001 -1.405e-001
Calcite           0.00    1.97    1.97   1.000e-001  1.000e-001  3.054e-005
K-Feldspar       -0.00   -0.27   -0.27   6.000e-001  7.405e-001  1.405e-001
Quartz            0.00   -4.23   -4.23   7.200e+001  8.915e+001  1.715e+001
SiO2(am)         -1.36   -4.23   -2.87   1.730e+001           0 -1.730e+001

-----------------------------Solution composition-----------------------------

      Elements          Molality       Moles

      Al             1.215e-008  1.750e-009
      C              1.756e-002  2.529e-003
      Ca             1.740e-005  2.506e-006
      Fe             3.456e-007  4.976e-008
      K              6.528e-004  9.401e-005
      Li             9.500e-014  1.368e-014
      Mg             1.500e-005  2.160e-006
      Na             1.122e+000  1.616e-001
      S              1.500e-005  2.160e-006
      Si             1.072e+000  1.543e-001

----------------------------Description of solution----------------------------

                                pH  =  12.069      Charge balance
                                pe  =   9.121      Adjusted to redox equilibrium
                     Activity of water  =   0.977
                        Ionic strength  =  2.226e+000
                     Mass of water (kg)  =  1.440e-001
                Total alkalinity (eq/kg)  =  1.123e+000
                     Total CO2 (mol/kg)  =  1.756e-002
                   Temperature (deg C)  =  15.500
                Electrical balance (eq)  = -4.190e-011
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
```

Iterations = 35
Total H = 1.639528e+001
Total O = 8.592254e+000

----------Distribution of species----------

| Species | Molality | Log Activity | Log Molality | Log Activity | Gamma |
|---|---|---|---|---|---|
| OH- | 8.118e-003 | 5.245e-003 | -2.091 | -2.280 | -0.190 |
| H+ | 9.605e-013 | 8.534e-013 | -12.018 | -12.069 | -0.051 |
| H2O | 5.553e+001 | 9.767e-001 | 1.744 | -0.010 | 0.000 |
| Al | 1.215e-008 | | | | |
| AlO2- | 1.134e-008 | 7.726e-009 | -7.945 | -8.112 | -0.167 |
| NaAlO2 | 8.106e-010 | 8.106e-010 | -9.091 | -9.091 | 0.000 |
| HAlO2 | 3.127e-014 | 3.127e-014 | -13.505 | -13.505 | 0.000 |
| Al(OH)2+ | 4.975e-020 | 3.389e-020 | -19.303 | -19.470 | -0.167 |
| AlOH+2 | 1.736e-025 | 2.432e-026 | -24.760 | -25.614 | -0.854 |
| Al+3 | 5.373e-032 | 3.653e-033 | -31.270 | -32.437 | -1.168 |
| AlSO4+ | 5.635e-036 | 3.839e-036 | -35.249 | -35.416 | -0.167 |
| Al(SO4)2- | 4.492e-040 | 3.060e-040 | -39.348 | -39.514 | -0.167 |
| Al2(OH)2+4 | 0.000e+000 | 0.000e+000 | -45.268 | -48.448 | -3.180 |
| Al3(OH)4+5 | 0.000e+000 | 0.000e+000 | -58.258 | -62.958 | -4.700 |
| Al13O4(OH)24+7 | 0.000e+000 | 0.000e+000 | -125.202 | -134.500 | -9.298 |
| C(-2) | 0.000e+000 | | | | |
| C2H4 | 0.000e+000 | 0.000e+000 | -284.089 | -284.089 | 0.000 |
| C(-3) | 0.000e+000 | | | | |
| C2H6 | 0.000e+000 | 0.000e+000 | -255.384 | -255.384 | 0.000 |
| C(-4) | 0.000e+000 | | | | |
| CH4 | 0.000e+000 | 0.000e+000 | -157.517 | -157.517 | 0.000 |
| C(2) | 0.000e+000 | | | | |
| CO | 0.000e+000 | 0.000e+000 | -57.742 | -57.742 | 0.000 |
| C(4) | 1.756e-002 | | | | |
| CO3-2 | 1.108e-002 | 1.553e-003 | -1.955 | -2.809 | -0.854 |
| NaCO3- | 6.376e-003 | 4.344e-003 | -2.195 | -2.362 | -0.167 |
| HCO3- | 5.348e-005 | 3.644e-005 | -4.272 | -4.438 | -0.167 |
| NaHCO3 | 3.907e-005 | 3.907e-005 | -4.408 | -4.408 | 0.000 |
| CaCO3 | 6.353e-006 | 6.353e-006 | -5.197 | -5.197 | 0.000 |
| MgCO3 | 4.495e-006 | 4.495e-006 | -5.347 | -5.347 | 0.000 |
| MgHCO3+ | 1.904e-009 | 1.297e-009 | -8.720 | -8.887 | -0.167 |
| CaHCO3+ | 1.381e-009 | 9.405e-010 | -8.860 | -9.027 | -0.167 |
| CO2 | 5.079e-011 | 8.492e-011 | -10.294 | -10.071 | 0.223 |
| FeCO3+ | 1.713e-026 | 1.167e-026 | -25.766 | -25.933 | -0.167 |
| FeCO3 | 6.314e-028 | 6.314e-028 | -27.200 | -27.200 | 0.000 |
| FeHCO3+ | 1.648e-031 | 1.123e-031 | -30.783 | -30.950 | -0.167 |
| Ca | 1.740e-005 | | | | |
| Ca+2 | 1.053e-005 | 2.209e-006 | -4.978 | -5.656 | -0.678 |
| CaCO3 | 6.353e-006 | 6.353e-006 | -5.197 | -5.197 | 0.000 |
| CaOH+ | 5.243e-007 | 3.572e-007 | -6.280 | -6.447 | -0.167 |
| CaHCO3+ | 1.381e-009 | 9.405e-010 | -8.860 | -9.027 | -0.167 |
| CaSO4 | 3.041e-010 | 3.041e-010 | -9.517 | -9.517 | 0.000 |
| Fe(2) | 1.324e-024 | | | | |
| Fe(OH)3- | 1.292e-024 | 8.800e-025 | -23.889 | -24.055 | -0.167 |
| Fe(OH)2 | 1.932e-026 | 1.932e-026 | -25.714 | -25.714 | 0.000 |
| Fe(OH)4-2 | 8.600e-027 | 1.007e-027 | -26.066 | -26.997 | -0.931 |
| FeOH+ | 3.119e-027 | 2.125e-027 | -26.506 | -26.673 | -0.167 |
| FeCO3 | 6.314e-028 | 6.314e-028 | -27.200 | -27.200 | 0.000 |
| Fe+2 | 2.797e-029 | 5.872e-030 | -28.553 | -29.231 | -0.678 |
| FeHCO3+ | 1.648e-031 | 1.123e-031 | -30.783 | -30.950 | -0.167 |
| FeSO4 | 9.557e-034 | 9.557e-034 | -33.020 | -33.020 | 0.000 |
| Fe(3) | 3.456e-007 | | | | |
| Fe(OH)4- | 3.448e-007 | 2.349e-007 | -6.462 | -6.629 | -0.167 |

| | | | | | |
|---|---|---|---|---|---|
| Fe(OH)3 | 8.171e-010 | 8.171e-010 | -9.088 | -9.088 | 0.000 |
| Fe(OH)2+ | 2.241e-015 | 1.526e-015 | -14.650 | -14.816 | -0.167 |
| FeOH+2 | 2.875e-023 | 4.028e-024 | -22.541 | -23.395 | -0.854 |
| FeCO3+ | 1.713e-026 | 1.167e-026 | -25.766 | -25.933 | -0.167 |
| Fe+3 | 8.018e-033 | 5.451e-034 | -32.096 | -33.263 | -1.168 |
| FeSO4+ | 5.545e-038 | 3.777e-038 | -37.256 | -37.423 | -0.167 |
| Fe(SO4)2- | 0.000e+000 | 0.000e+000 | -41.860 | -42.027 | -0.167 |
| Fe2(OH)2+4 | 0.000e+000 | 0.000e+000 | -42.180 | -45.360 | -3.180 |
| Fe3(OH)4+5 | 0.000e+000 | 0.000e+000 | -53.156 | -57.856 | -4.700 |
| H(0) | 0.000e+000 | | | | |
| H2 | 0.000e+000 | 0.000e+000 | -45.901 | -45.678 | 0.223 |
| K | 6.528e-004 | | | | |
| K+ | 6.513e-004 | 3.950e-004 | -3.186 | -3.403 | -0.217 |
| KOH | 1.567e-006 | 1.567e-006 | -5.805 | -5.805 | 0.000 |
| KSO4- | 4.619e-009 | 3.146e-009 | -8.335 | -8.502 | -0.167 |
| KHSO4 | 1.662e-021 | 1.662e-021 | -20.779 | -20.779 | 0.000 |
| Li | 9.500e-014 | | | | |
| Li+ | 9.308e-014 | 7.337e-014 | -13.031 | -13.135 | -0.103 |
| LiOH | 1.923e-015 | 1.923e-015 | -14.716 | -14.716 | 0.000 |
| LiSO4- | 6.513e-019 | 4.437e-019 | -18.186 | -18.353 | -0.167 |
| Mg | 1.500e-005 | | | | |
| Mg+2 | 1.051e-005 | 3.133e-006 | -4.979 | -5.504 | -0.525 |
| MgCO3 | 4.495e-006 | 4.495e-006 | -5.347 | -5.347 | 0.000 |
| MgHCO3+ | 1.904e-009 | 1.297e-009 | -8.720 | -8.887 | -0.167 |
| MgSO4 | 6.688e-010 | 6.688e-010 | -9.175 | -9.175 | 0.000 |
| Mg4(OH)4+4 | 4.443e-011 | 2.938e-014 | -10.352 | -13.532 | -3.180 |
| Na | 1.122e+000 | | | | |
| Na+ | 9.179e-001 | 6.253e-001 | -0.037 | -0.204 | -0.167 |
| NaHSiO3 | 1.972e-001 | 1.972e-001 | -0.705 | -0.705 | 0.000 |
| NaCO3- | 6.376e-003 | 4.344e-003 | -2.195 | -2.362 | -0.167 |
| NaOH | 5.791e-004 | 5.791e-004 | -3.237 | -3.237 | 0.000 |
| NaHCO3 | 3.907e-005 | 3.907e-005 | -4.408 | -4.408 | 0.000 |
| NaSO4- | 6.228e-006 | 4.243e-006 | -5.206 | -5.372 | -0.167 |
| NaAlO2 | 8.106e-010 | 8.106e-010 | -9.091 | -9.091 | 0.000 |
| O(0) | 1.114e-004 | | | | |
| O2 | 5.571e-005 | 9.314e-005 | -4.254 | -4.031 | 0.223 |
| S(-2) | 0.000e+000 | | | | |
| HS- | 0.000e+000 | 0.000e+000 | -153.084 | -153.274 | -0.190 |
| S-2 | 0.000e+000 | 0.000e+000 | -153.630 | -154.416 | -0.787 |
| H2S | 0.000e+000 | 0.000e+000 | -158.200 | -158.200 | 0.000 |
| S2-2 | 0.000e+000 | 0.000e+000 | -273.113 | -274.044 | -0.931 |
| S3-2 | 0.000e+000 | 0.000e+000 | -392.778 | -393.709 | -0.931 |
| S4-2 | 0.000e+000 | 0.000e+000 | -512.674 | -513.606 | -0.931 |
| S5-2 | 0.000e+000 | 0.000e+000 | -632.796 | -633.727 | -0.931 |
| S(2) | 0.000e+000 | | | | |
| S2O3-2 | 0.000e+000 | 0.000e+000 | -165.515 | -166.446 | -0.931 |
| HS2O3- | 0.000e+000 | 0.000e+000 | -177.334 | -177.501 | -0.167 |
| S(3) | 0.000e+000 | | | | |
| S2O4-2 | 0.000e+000 | 0.000e+000 | -151.952 | -152.739 | -0.787 |
| S(4) | 0.000e+000 | | | | |
| SO3-2 | 0.000e+000 | 0.000e+000 | -51.281 | -52.135 | -0.854 |
| HSO3- | 0.000e+000 | 0.000e+000 | -56.856 | -57.023 | -0.167 |
| H2SO3 | 0.000e+000 | 0.000e+000 | -67.059 | -67.059 | 0.000 |
| SO2 | 0.000e+000 | 0.000e+000 | -67.295 | -67.295 | 0.000 |
| S2O6-2 | 0.000e+000 | 0.000e+000 | -86.580 | -87.511 | -0.931 |
| S3O6-2 | 0.000e+000 | 0.000e+000 | -208.772 | -209.703 | -0.931 |
| S4O6-2 | 0.000e+000 | 0.000e+000 | -314.717 | -315.648 | -0.931 |
| S5O6-2 | 0.000e+000 | 0.000e+000 | -450.135 | -451.066 | -0.931 |
| S(5) | 0.000e+000 | | | | |
| S2O5-2 | 0.000e+000 | 0.000e+000 | -117.915 | -118.846 | -0.931 |
| S(6) | 1.500e-005 | | | | |
| SO4-2 | 8.769e-006 | 1.027e-006 | -5.057 | -5.988 | -0.931 |

```
   NaSO4-              6.228e-006  4.243e-006    -5.206    -5.372    -0.167
   KSO4-               4.619e-009  3.146e-009    -8.335    -8.502    -0.167
   MgSO4               6.688e-010  6.688e-010    -9.175    -9.175     0.000
   CaSO4               3.041e-010  3.041e-010    -9.517    -9.517     0.000
   HSO4-               9.948e-017  6.777e-017   -16.002   -16.169    -0.167
   LiSO4-              6.513e-019  4.437e-019   -18.186   -18.353    -0.167
   KHSO4               1.662e-021  1.662e-021   -20.779   -20.779     0.000
   H2SO4               7.128e-032  7.128e-032   -31.147   -31.147     0.000
   FeSO4               9.557e-034  9.557e-034   -33.020   -33.020     0.000
   AlSO4+              5.635e-036  3.839e-036   -35.249   -35.416    -0.167
   FeSO4+              5.545e-038  3.777e-038   -37.256   -37.423    -0.167
   Al(SO4)2-           4.492e-040  3.060e-040   -39.348   -39.514    -0.167
   Fe(SO4)2-           0.000e+000  0.000e+000   -41.860   -42.027    -0.167
S(7)          0.000e+000
   S2O8-2              0.000e+000  0.000e+000   -60.765   -61.697    -0.931
S(8)          1.066e-038
   HSO5-               1.066e-038  7.260e-039   -37.972   -38.139    -0.167
Si            1.072e+000
   H4(H2SiO4)4-4       2.148e-001  2.197e-005    -0.668    -4.658    -3.990
   NaHSiO3             1.972e-001  1.972e-001    -0.705    -0.705     0.000
   HSiO3-              8.167e-003  5.564e-003    -2.088    -2.255    -0.167
   H2SiO4-2            7.256e-003  8.497e-004    -2.139    -3.071    -0.931
   SiO2                5.917e-005  5.917e-005    -4.228    -4.228     0.000
   H6(H2SiO4)4-2       2.726e-006  3.193e-007    -5.564    -6.496    -0.931
```

## File 20. Fresh Cement, Maximum ions, 95%/5% Mixing Ratio

*INPUT FILE*

```
SOLUTION 1
    temp      15
    pH        7.5 charge
    pe        4
    redox     pe
    units     mmol/kgw
    density   1
    Alkalinity 0
    Cl(-1)    7.5
    Li        1e-010
    Al        1e-010
    Ca        3.1
    Mg        5
    Na        18
    K         1.9
    S(6)      7.3
    N(5)      7.9
    C(4)      21.8
    Br(-1)    0
    Si        0.01
    -water    0.144 # kg

EQUILIBRIUM_PHASES 1
    Brucite   0 0.208
    Ca(OH)2*(CSH(1.5)) 0 1.42
    Calcite   0 0.001
    CSH(1.0-2.5) 0 2.386
    Ettringite 0 0.016
    Gibbsite  0 0.001
    Goethite  0 0.001
    Hydrogarnet(C3AH6) 0 0.384
    SiO2(am)  0 0.02
    KOH(cement) 0 0.148
```

```
    NaOH(cement) 0 0.022
    Monosulfate 0 0.192
GAS_PHASE 1
    -fixed_pressure
    -pressure 1
    -volume 1
    -temperature 25
    CO2(g)    0.056
SAVE solution 1-1
END
SOLUTION 2
    temp      25
    pH        7.5 charge
    pe        4
    redox     pe
    units     mmol/kgs
    density   1
    Li        0
    Alkalinity 0
    Ca        3.1
    Mg        5
    Na        18
    C(4)      21.8
    Cl        7.5
    S(6)      7.3
    N(5)      7.8
    Si        0.001
    K         1.9
    -water    0.144 # kg
GAS_PHASE 2
    -fixed_pressure
    -pressure 1
    -volume 1
    -temperature 25
    CO2(g)    0.056
    O2(g)     0.18
EQUILIBRIUM_PHASES 2
    calcite   0 1
SAVE solution 2-2
END
MIX 1
    1    0.95
    2    0.05
EQUILIBRIUM_PHASES 3
    Albite    0 0.6
    Calcite   0 0.1
    K-Feldspar 0 0.6
    Quartz    0 72
    SiO2(am)  0 17.3
```

### *Sample Output, Final Time Step (file 20)*

```
-------------------------------------------
Beginning of batch-reaction calculations.
-------------------------------------------

Reaction step 1.

Using mix 1.
Using pure phase assemblage 3.

Mixture 1.
```

9.500e-001 Solution 1 Solution after simulation 1.
5.000e-002 Solution 2 Solution after simulation 2.

----------Phase assemblage----------

| Phase | SI | log IAP | log KT | Moles in assemblage Initial | Final | Delta |
|---|---|---|---|---|---|---|
| Albite | -0.00 | 2.93 | 2.93 | 6.000e-001 | 4.592e-001 | -1.408e-001 |
| Calcite | 0.00 | 1.97 | 1.97 | 1.000e-001 | 1.001e-001 | 5.206e-005 |
| K-Feldspar | -0.00 | -0.27 | -0.27 | 6.000e-001 | 7.408e-001 | 1.408e-001 |
| Quartz | 0.00 | -4.23 | -4.23 | 7.200e+001 | 8.915e+001 | 1.715e+001 |
| SiO2(am) | -1.36 | -4.23 | -2.87 | 1.730e+001 | 0 | -1.730e+001 |

----------Solution composition----------

| Elements | Molality | Moles |
|---|---|---|
| Al | 1.195e-008 | 1.721e-009 |
| C | 1.816e-002 | 2.615e-003 |
| Ca | 1.724e-005 | 2.481e-006 |
| Cl | 7.504e-003 | 1.080e-003 |
| Fe | 3.457e-007 | 4.976e-008 |
| K | 6.639e-004 | 9.557e-005 |
| Li | 9.503e-014 | 1.368e-014 |
| Mg | 2.509e-004 | 3.611e-005 |
| N | 7.899e-003 | 1.137e-003 |
| Na | 1.141e+000 | 1.643e-001 |
| S | 3.663e-004 | 5.273e-005 |
| Si | 1.074e+000 | 1.546e-001 |

----------Description of solution----------

pH = 12.068 Charge balance
pe = 9.101 Adjusted to redox equilibrium
Activity of water = 0.976
Ionic strength = 2.241e+000
Mass of water (kg) = 1.440e-001
Total alkalinity (eq/kg) = 1.126e+000
Total CO2 (mol/kg) = 1.816e-002
Temperature (deg C) = 15.500
Electrical balance (eq) = -1.106e-013
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.00
Iterations = 23
Total H = 1.639003e+001
Total O = 8.594147e+000

----------Distribution of species----------

| Species | Molality | Log Activity | Log Molality | Log Activity | Gamma |
|---|---|---|---|---|---|
| OH- | 8.098e-003 | 5.235e-003 | -2.092 | -2.281 | -0.189 |
| H+ | 9.607e-013 | 8.546e-013 | -12.017 | -12.068 | -0.051 |
| H2O | 5.553e+001 | 9.761e-001 | 1.744 | -0.011 | 0.000 |
| Al | 1.195e-008 | | | | |
| AlO2- | 1.114e-008 | 7.596e-009 | -7.953 | -8.119 | -0.166 |
| NaAlO2 | 8.106e-010 | 8.106e-010 | -9.091 | -9.091 | 0.000 |
| HAlO2 | 3.078e-014 | 3.078e-014 | -13.512 | -13.512 | 0.000 |
| Al(OH)2+ | 4.901e-020 | 3.341e-020 | -19.310 | -19.476 | -0.166 |
| AlOH+2 | 1.716e-025 | 2.402e-026 | -24.765 | -25.619 | -0.854 |

| | | | | | |
|---|---|---|---|---|---|
| Al+3 | 5.319e-032 | 3.615e-033 | -31.274 | -32.442 | -1.168 |
| AlSO4+ | 1.349e-034 | 9.199e-035 | -33.870 | -34.036 | -0.166 |
| Al(SO4)2- | 2.605e-037 | 1.776e-037 | -36.584 | -36.751 | -0.166 |
| Al2(OH)2+4 | 0.000e+000 | 0.000e+000 | -45.277 | -48.458 | -3.182 |
| Al3(OH)4+5 | 0.000e+000 | 0.000e+000 | -58.271 | -62.975 | -4.704 |
| Al13O4(OH)24+7 | 0.000e+000 | 0.000e+000 | -125.280 | -134.585 | -9.305 |
| C(-2) | 0.000e+000 | | | | |
| C2H4 | 0.000e+000 | 0.000e+000 | -283.824 | -283.824 | 0.000 |
| C(-3) | 0.000e+000 | | | | |
| C2H6 | 0.000e+000 | 0.000e+000 | -255.079 | -255.079 | 0.000 |
| C(-4) | 0.000e+000 | | | | |
| CH4 | 0.000e+000 | 0.000e+000 | -157.344 | -157.344 | 0.000 |
| C(2) | 0.000e+000 | | | | |
| CO | 0.000e+000 | 0.000e+000 | -57.690 | -57.690 | 0.000 |
| C(4) | 1.816e-002 | | | | |
| CO3-2 | 1.135e-002 | 1.590e-003 | -1.945 | -2.799 | -0.854 |
| NaCO3- | 6.634e-003 | 4.522e-003 | -2.178 | -2.345 | -0.166 |
| MgCO3 | 7.287e-005 | 7.287e-005 | -4.137 | -4.137 | 0.000 |
| HCO3- | 5.478e-005 | 3.734e-005 | -4.261 | -4.428 | -0.166 |
| NaHCO3 | 4.073e-005 | 4.073e-005 | -4.390 | -4.390 | 0.000 |
| CaCO3 | 6.353e-006 | 6.353e-006 | -5.197 | -5.197 | 0.000 |
| MgHCO3+ | 3.088e-008 | 2.105e-008 | -7.510 | -7.677 | -0.166 |
| CaHCO3+ | 1.381e-009 | 9.418e-010 | -8.860 | -9.026 | -0.166 |
| CO2 | 5.199e-011 | 8.720e-011 | -10.284 | -10.059 | 0.225 |
| FeCO3+ | 1.767e-026 | 1.205e-026 | -25.753 | -25.919 | -0.166 |
| FeCO3 | 6.819e-028 | 6.819e-028 | -27.166 | -27.166 | 0.000 |
| FeHCO3+ | 1.781e-031 | 1.214e-031 | -30.749 | -30.916 | -0.166 |
| Ca | 1.724e-005 | | | | |
| Ca+2 | 1.028e-005 | 2.159e-006 | -4.988 | -5.666 | -0.678 |
| CaCO3 | 6.353e-006 | 6.353e-006 | -5.197 | -5.197 | 0.000 |
| CaOH+ | 5.108e-007 | 3.483e-007 | -6.292 | -6.458 | -0.166 |
| CaNO3+ | 7.605e-008 | 5.184e-008 | -7.119 | -7.285 | -0.166 |
| CaSO4 | 7.193e-009 | 7.193e-009 | -8.143 | -8.143 | 0.000 |
| CaCl+ | 2.803e-009 | 1.911e-009 | -8.552 | -8.719 | -0.166 |
| CaHCO3+ | 1.381e-009 | 9.418e-010 | -8.860 | -9.026 | -0.166 |
| CaCl2 | 1.066e-011 | 1.066e-011 | -10.972 | -10.972 | 0.000 |
| Cl(-1) | 7.504e-003 | | | | |
| Cl- | 7.058e-003 | 4.282e-003 | -2.151 | -2.368 | -0.217 |
| NaCl | 4.454e-004 | 4.454e-004 | -3.351 | -3.351 | 0.000 |
| MgCl+ | 2.467e-007 | 1.682e-007 | -6.608 | -6.774 | -0.166 |
| KCl | 4.745e-008 | 4.745e-008 | -7.324 | -7.324 | 0.000 |
| CaCl+ | 2.803e-009 | 1.911e-009 | -8.552 | -8.719 | -0.166 |
| CaCl2 | 1.066e-011 | 1.066e-011 | -10.972 | -10.972 | 0.000 |
| HCl | 8.077e-016 | 8.077e-016 | -15.093 | -15.093 | 0.000 |
| LiCl | 9.643e-018 | 9.643e-018 | -17.016 | -17.016 | 0.000 |
| FeCl+ | 2.729e-032 | 1.860e-032 | -31.564 | -31.730 | -0.166 |
| FeCl2+ | 1.995e-036 | 1.360e-036 | -35.700 | -35.866 | -0.166 |
| FeCl+2 | 1.722e-036 | 2.410e-037 | -35.764 | -36.618 | -0.854 |
| FeCl2 | 4.073e-037 | 4.073e-037 | -36.390 | -36.390 | 0.000 |
| FeCl4-2 | 1.819e-040 | 0.000e+000 | -39.740 | -40.672 | -0.932 |
| FeCl4- | 0.000e+000 | 0.000e+000 | -43.357 | -43.523 | -0.166 |
| Cl(1) | 1.775e-020 | | | | |
| ClO- | 1.775e-020 | 1.210e-020 | -19.751 | -19.917 | -0.166 |
| HClO | 3.835e-025 | 3.835e-025 | -24.416 | -24.416 | 0.000 |
| Cl(3) | 8.207e-031 | | | | |
| ClO2- | 8.207e-031 | 5.595e-031 | -30.086 | -30.252 | -0.166 |
| HClO2 | 7.069e-040 | 7.069e-040 | -39.151 | -39.151 | 0.000 |
| Cl(5) | 8.091e-027 | | | | |
| ClO3- | 8.091e-027 | 5.231e-027 | -26.092 | -26.281 | -0.189 |
| Cl(7) | 3.201e-027 | | | | |
| ClO4- | 3.201e-027 | 2.070e-027 | -26.495 | -26.684 | -0.189 |
| Fe(2) | 1.387e-024 | | | | |

| | | | | | |
|---|---|---|---|---|---|
| Fe(OH)3- | 1.354e-024 | 9.231e-025 | -23.868 | -24.035 | -0.166 |
| Fe(OH)2 | 2.030e-026 | 2.030e-026 | -25.692 | -25.692 | 0.000 |
| Fe(OH)4-2 | 9.015e-027 | 1.054e-027 | -26.045 | -26.977 | -0.932 |
| FeOH+ | 3.282e-027 | 2.238e-027 | -26.484 | -26.650 | -0.166 |
| FeCO3 | 6.819e-028 | 6.819e-028 | -27.166 | -27.166 | 0.000 |
| Fe+2 | 2.952e-029 | 6.195e-030 | -28.530 | -29.208 | -0.678 |
| FeHCO3+ | 1.781e-031 | 1.214e-031 | -30.749 | -30.916 | -0.166 |
| FeCl+ | 2.729e-032 | 1.860e-032 | -31.564 | -31.730 | -0.166 |
| FeSO4 | 2.442e-032 | 2.442e-032 | -31.612 | -31.612 | 0.000 |
| FeCl2 | 4.073e-037 | 4.073e-037 | -36.390 | -36.390 | 0.000 |
| FeCl4-2 | 1.819e-040 | 0.000e+000 | -39.740 | -40.672 | -0.932 |
| Fe(3) | 3.457e-007 | | | | |
| Fe(OH)4- | 3.448e-007 | 2.351e-007 | -6.462 | -6.629 | -0.166 |
| Fe(OH)3 | 8.194e-010 | 8.194e-010 | -9.087 | -9.087 | 0.000 |
| Fe(OH)2+ | 2.250e-015 | 1.534e-015 | -14.648 | -14.814 | -0.166 |
| FeOH+2 | 2.897e-023 | 4.055e-024 | -22.538 | -23.392 | -0.854 |
| FeCO3+ | 1.767e-026 | 1.205e-026 | -25.753 | -25.919 | -0.166 |
| Fe+3 | 8.091e-033 | 5.499e-034 | -32.092 | -33.260 | -1.168 |
| FeNO3+2 | 1.882e-034 | 2.635e-035 | -33.725 | -34.579 | -0.854 |
| FeCl2+ | 1.995e-036 | 1.360e-036 | -35.700 | -35.866 | -0.166 |
| FeCl+2 | 1.722e-036 | 2.410e-037 | -35.764 | -36.618 | -0.854 |
| FeSO4+ | 1.353e-036 | 9.226e-037 | -35.869 | -36.035 | -0.166 |
| Fe(SO4)2- | 8.159e-040 | 5.562e-040 | -39.088 | -39.255 | -0.166 |
| Fe2(OH)2+4 | 0.000e+000 | 0.000e+000 | -42.172 | -45.354 | -3.182 |
| FeCl4- | 0.000e+000 | 0.000e+000 | -43.357 | -43.523 | -0.166 |
| FeNO2+2 | 0.000e+000 | 0.000e+000 | -45.304 | -46.157 | -0.854 |
| Fe3(OH)4+5 | 0.000e+000 | 0.000e+000 | -53.144 | -57.848 | -4.704 |
| H(0) | 0.000e+000 | | | | |
| H2 | 0.000e+000 | 0.000e+000 | -45.862 | -45.638 | 0.225 |
| K | 6.639e-004 | | | | |
| K+ | 6.622e-004 | 4.017e-004 | -3.179 | -3.396 | -0.217 |
| KOH | 1.591e-006 | 1.591e-006 | -5.798 | -5.798 | 0.000 |
| KSO4- | 1.137e-007 | 7.749e-008 | -6.944 | -7.111 | -0.166 |
| KCl | 4.745e-008 | 4.745e-008 | -7.324 | -7.324 | 0.000 |
| KHSO4 | 4.100e-020 | 4.100e-020 | -19.387 | -19.387 | 0.000 |
| Li | 9.503e-014 | | | | |
| Li+ | 9.308e-014 | 7.345e-014 | -13.031 | -13.134 | -0.103 |
| LiOH | 1.922e-015 | 1.922e-015 | -14.716 | -14.716 | 0.000 |
| LiSO4- | 1.578e-017 | 1.075e-017 | -16.802 | -16.968 | -0.166 |
| LiCl | 9.643e-018 | 9.643e-018 | -17.016 | -17.016 | 0.000 |
| Mg | 2.509e-004 | | | | |
| Mg+2 | 1.663e-004 | 4.962e-005 | -3.779 | -4.304 | -0.525 |
| MgCO3 | 7.287e-005 | 7.287e-005 | -4.137 | -4.137 | 0.000 |
| Mg4(OH)4+4 | 2.789e-006 | 1.835e-009 | -5.555 | -8.736 | -3.182 |
| MgSO4 | 2.565e-007 | 2.565e-007 | -6.591 | -6.591 | 0.000 |
| MgCl+ | 2.467e-007 | 1.682e-007 | -6.608 | -6.774 | -0.166 |
| MgHCO3+ | 3.088e-008 | 2.105e-008 | -7.510 | -7.677 | -0.166 |
| N(-03) | 0.000e+000 | | | | |
| N3- | 0.000e+000 | 0.000e+000 | -106.951 | -107.118 | -0.166 |
| HN3 | 0.000e+000 | 0.000e+000 | -114.396 | -114.396 | 0.000 |
| N(-3) | 0.000e+000 | | | | |
| NH3 | 0.000e+000 | 0.000e+000 | -70.465 | -70.465 | 0.000 |
| NH4+ | 0.000e+000 | 0.000e+000 | -72.744 | -72.995 | -0.251 |
| NH4SO4- | 0.000e+000 | 0.000e+000 | -86.031 | -86.197 | -0.166 |
| N(0) | 4.486e-027 | | | | |
| N2 | 2.243e-027 | 2.243e-027 | -26.649 | -26.649 | 0.000 |
| N(3) | 1.477e-016 | | | | |
| NO2- | 1.477e-016 | 8.959e-017 | -15.831 | -16.048 | -0.217 |
| HNO2 | 1.601e-025 | 1.601e-025 | -24.796 | -24.796 | 0.000 |
| FeNO2+2 | 0.000e+000 | 0.000e+000 | -45.304 | -46.157 | -0.854 |
| N(5) | 7.899e-003 | | | | |
| NO3- | 7.899e-003 | 4.792e-003 | -2.102 | -2.319 | -0.217 |

| | | | | | |
|---|---|---|---|---|---|
| CaNO3+ | 7.605e-008 | 5.184e-008 | -7.119 | -7.285 | -0.166 |
| HNO3 | 1.705e-016 | 1.705e-016 | -15.768 | -15.768 | 0.000 |
| FeNO3+2 | 1.882e-034 | 2.635e-035 | -33.725 | -34.579 | -0.854 |
| Na | 1.141e+000 | | | | |
| Na+ | 9.330e-001 | 6.360e-001 | -0.030 | -0.197 | -0.166 |
| NaHSiO3 | 2.002e-001 | 2.002e-001 | -0.699 | -0.699 | 0.000 |
| NaCO3- | 6.634e-003 | 4.522e-003 | -2.178 | -2.345 | -0.166 |
| NaOH | 5.879e-004 | 5.879e-004 | -3.231 | -3.231 | 0.000 |
| NaCl | 4.454e-004 | 4.454e-004 | -3.351 | -3.351 | 0.000 |
| NaSO4- | 1.533e-004 | 1.045e-004 | -3.815 | -3.981 | -0.166 |
| NaHCO3 | 4.073e-005 | 4.073e-005 | -4.390 | -4.390 | 0.000 |
| NaAlO2 | 8.106e-010 | 8.106e-010 | -9.091 | -9.091 | 0.000 |
| O(0) | 9.215e-005 | | | | |
| O2 | 4.608e-005 | 7.729e-005 | -4.337 | -4.112 | 0.225 |
| S(-2) | 0.000e+000 | | | | |
| HS- | 0.000e+000 | 0.000e+000 | -151.538 | -151.727 | -0.189 |
| S-2 | 0.000e+000 | 0.000e+000 | -152.083 | -152.870 | -0.787 |
| H2S | 0.000e+000 | 0.000e+000 | -156.652 | -156.652 | 0.000 |
| S2-2 | 0.000e+000 | 0.000e+000 | -270.059 | -270.991 | -0.932 |
| S3-2 | 0.000e+000 | 0.000e+000 | -388.218 | -389.149 | -0.932 |
| S4-2 | 0.000e+000 | 0.000e+000 | -506.607 | -507.539 | -0.932 |
| S5-2 | 0.000e+000 | 0.000e+000 | -625.221 | -626.153 | -0.932 |
| S(2) | 0.000e+000 | | | | |
| S2O3-2 | 0.000e+000 | 0.000e+000 | -162.583 | -163.515 | -0.932 |
| HS2O3- | 0.000e+000 | 0.000e+000 | -174.403 | -174.569 | -0.166 |
| S(3) | 0.000e+000 | | | | |
| S2O4-2 | 0.000e+000 | 0.000e+000 | -149.061 | -149.848 | -0.787 |
| S(4) | 0.000e+000 | | | | |
| SO3-2 | 0.000e+000 | 0.000e+000 | -49.857 | -50.710 | -0.854 |
| HSO3- | 0.000e+000 | 0.000e+000 | -55.431 | -55.598 | -0.166 |
| H2SO3 | 0.000e+000 | 0.000e+000 | -65.634 | -65.634 | 0.000 |
| SO2 | 0.000e+000 | 0.000e+000 | -65.869 | -65.869 | 0.000 |
| S2O6-2 | 0.000e+000 | 0.000e+000 | -83.769 | -84.701 | -0.932 |
| S3O6-2 | 0.000e+000 | 0.000e+000 | -204.454 | -205.386 | -0.932 |
| S4O6-2 | 0.000e+000 | 0.000e+000 | -308.892 | -309.824 | -0.932 |
| S5O6-2 | 0.000e+000 | 0.000e+000 | -442.803 | -443.735 | -0.932 |
| S(5) | 0.000e+000 | | | | |
| S2O5-2 | 0.000e+000 | 0.000e+000 | -115.064 | -115.996 | -0.932 |
| S(6) | 3.663e-004 | | | | |
| SO4-2 | 2.126e-004 | 2.487e-005 | -3.672 | -4.604 | -0.932 |
| NaSO4- | 1.533e-004 | 1.045e-004 | -3.815 | -3.981 | -0.166 |
| MgSO4 | 2.565e-007 | 2.565e-007 | -6.591 | -6.591 | 0.000 |
| KSO4- | 1.137e-007 | 7.749e-008 | -6.944 | -7.111 | -0.166 |
| CaSO4 | 7.193e-009 | 7.193e-009 | -8.143 | -8.143 | 0.000 |
| HSO4- | 2.410e-015 | 1.643e-015 | -14.618 | -14.784 | -0.166 |
| LiSO4- | 1.578e-017 | 1.075e-017 | -16.802 | -16.968 | -0.166 |
| KHSO4 | 4.100e-020 | 4.100e-020 | -19.387 | -19.387 | 0.000 |
| H2SO4 | 1.731e-030 | 1.731e-030 | -29.762 | -29.762 | 0.000 |
| FeSO4 | 2.442e-032 | 2.442e-032 | -31.612 | -31.612 | 0.000 |
| AlSO4+ | 1.349e-034 | 9.199e-035 | -33.870 | -34.036 | -0.166 |
| FeSO4+ | 1.353e-036 | 9.226e-037 | -35.869 | -36.035 | -0.166 |
| Al(SO4)2- | 2.605e-037 | 1.776e-037 | -36.584 | -36.751 | -0.166 |
| Fe(SO4)2- | 8.159e-040 | 5.562e-040 | -39.088 | -39.255 | -0.166 |
| NH4SO4- | 0.000e+000 | 0.000e+000 | -86.031 | -86.197 | -0.166 |
| S(7) | 0.000e+000 | | | | |
| S2O8-2 | 0.000e+000 | 0.000e+000 | -58.036 | -58.968 | -0.932 |
| S(8) | 2.352e-037 | | | | |
| HSO5- | 2.352e-037 | 1.604e-037 | -36.628 | -36.795 | -0.166 |
| Si | 1.074e+000 | | | | |
| H4(H2SiO4)4-4 | 2.146e-001 | 2.175e-005 | -0.668 | -4.663 | -3.994 |
| NaHSiO3 | 2.002e-001 | 2.002e-001 | -0.699 | -0.699 | 0.000 |
| HSiO3- | 8.146e-003 | 5.553e-003 | -2.089 | -2.255 | -0.166 |

```
H2SiO4-2            7.237e-003  8.465e-004    -2.140    -3.072    -0.932
SiO2                5.917e-005  5.917e-005    -4.228    -4.228     0.000
H6(H2SiO4)4-2       2.709e-006  3.169e-007    -5.567    -6.499    -0.932
```

## File 21. Fresh Cement, Minimum ions, 50%/50% Mixing Ratio

*INPUT FILE*

```
SOLUTION 1
   temp      15
   pH        7.5 charge
   pe        4
   redox     pe
   units     mmol/kgw
   density   1
   Alkalinity 0
   Cl(-1)    0
   Li        1e-010
   Al        1e-010
   Ca        0.6
   Mg        0.3
   Na        1.3
   K         0
   S(6)      0.3
   N(5)      0
   C(4)      1.4
   Br(-1)    0
   Si        0.01
   -water    0.144 # kg

EQUILIBRIUM_PHASES 1
   Brucite   0 0.208
   Ca(OH)2*(CSH(1.5)) 0 1.42
   Calcite   0 0.001
   CSH(1.0-2.5) 0 2.386
   Ettringite 0 0.016
   Gibbsite  0 0.001
   Goethite  0 0.001
   Hydrogarnet(C3AH6) 0 0.384
   SiO2(am)  0 0.02
   KOH(cement) 0 0.148
   NaOH(cement) 0 0.022
   Monosulfate 0 0.192
GAS_PHASE 1
   -fixed_pressure
   -pressure 1
   -volume 1
   -temperature 25
   CO2(g)    0.056
SAVE solution 1-1
END
SOLUTION 2
   temp      25
   pH        7.5 charge
   pe        4
   redox     pe
   units     mmol/kgs
   density   1
   Li        0
   Alkalinity 0
   Ca        0.6
   Mg        0.3
```

```
    Na       1.3
    C(4)     1.4
    Cl       0
    S(6)     0.3
    N(5)     0
    Si       0.001
    K        0
    -water   0.144 # kg
GAS_PHASE 2
    -fixed_pressure
    -pressure 1
    -volume 1
    -temperature 25
    CO2(g)   0.056
    O2(g)    0.18
EQUILIBRIUM_PHASES 2
    calcite  0 1
SAVE solution 2-2
END
MIX 1
    1   0.5
    2   0.5
EQUILIBRIUM_PHASES 3
    Albite   0 0.6
    Calcite  0 0.1
    K-Feldspar 0 0.6
    Quartz   0 72
    SiO2(am)  0 17.3
```

*SAMPLE OUTPUT, FINAL TIME STEP (FILE 21)*

```
-------------------------------------------
Beginning of batch-reaction calculations.
-------------------------------------------

Reaction step 1.

Using mix 1.
Using pure phase assemblage 3.

Mixture 1.

      5.000e-001 Solution 1       Solution after simulation 1.
      5.000e-001 Solution 2       Solution after simulation 2.

-------------------------------Phase assemblage--------------------------------

                                        Moles in assemblage
Phase              SI log IAP  log KT      Initial       Final       Delta

Albite            0.00    2.80    2.80   6.000e-001  5.261e-001 -7.394e-002
Calcite           0.00    1.90    1.90   1.000e-001  1.003e-001  2.686e-004
K-Feldspar        0.00   -0.32   -0.32   6.000e-001  6.739e-001  7.394e-002
Quartz            0.00   -4.13   -4.13   7.200e+001  8.922e+001  1.722e+001
SiO2(am)         -1.32   -4.13   -2.81   1.730e+001           0 -1.730e+001

-----------------------------Solution composition------------------------------

      Elements          Molality       Moles

      Al              2.915e-008  4.201e-009
      C               1.369e-002  1.972e-003
```

| | | |
|---|---|---|
| Ca | 1.565e-005 | 2.255e-006 |
| Fe | 1.818e-007 | 2.619e-008 |
| K | 3.932e-004 | 5.665e-005 |
| Li | 4.997e-014 | 7.200e-015 |
| Mg | 1.499e-004 | 2.160e-005 |
| Na | 5.907e-001 | 8.512e-002 |
| S | 1.499e-004 | 2.160e-005 |
| Si | 5.481e-001 | 7.898e-002 |

----------Description of solution----------

pH = 11.992 Charge balance
pe = 9.083 Adjusted to redox equilibrium
Activity of water = 0.988
Ionic strength = 1.121e+000
Mass of water (kg) = 1.441e-001
Total alkalinity (eq/kg) = 5.912e-001
Total CO2 (mol/kg) = 1.369e-002
Temperature (deg C) = 20.000
Electrical balance (eq) = -2.229e-011
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.00
Iterations = 28
Total H = 1.620397e+001
Total O = 8.306725e+000

----------Distribution of species----------

| Species | Molality | Log Activity | Log Molality | Log Activity | Gamma |
|---|---|---|---|---|---|
| OH- | 1.004e-002 | 6.369e-003 | -1.998 | -2.196 | -0.198 |
| H+ | 1.239e-012 | 1.018e-012 | -11.907 | -11.992 | -0.085 |
| H2O | 5.553e+001 | 9.875e-001 | 1.744 | -0.005 | 0.000 |
| Al | 2.915e-008 | | | | |
| AlO2- | 2.811e-008 | 1.858e-008 | -7.551 | -7.731 | -0.180 |
| NaAlO2 | 1.039e-009 | 1.039e-009 | -8.983 | -8.983 | 0.000 |
| HAlO2 | 7.086e-014 | 7.086e-014 | -13.150 | -13.150 | 0.000 |
| Al(OH)2+ | 1.032e-019 | 6.818e-020 | -18.986 | -19.166 | -0.180 |
| AlOH+2 | 2.632e-025 | 4.230e-026 | -24.580 | -25.374 | -0.794 |
| Al+3 | 7.347e-032 | 5.476e-033 | -31.134 | -32.262 | -1.128 |
| AlSO4+ | 1.233e-034 | 8.150e-035 | -33.909 | -34.089 | -0.180 |
| Al(SO4)2- | 1.393e-037 | 9.203e-038 | -36.856 | -37.036 | -0.180 |
| Al2(OH)2+4 | 0.000e+000 | 0.000e+000 | -45.329 | -48.240 | -2.911 |
| Al3(OH)4+5 | 0.000e+000 | 0.000e+000 | -58.405 | -62.718 | -4.313 |
| Al13O4(OH)24+7 | 0.000e+000 | 0.000e+000 | -126.037 | -134.535 | -8.498 |
| C(-2) | 0.000e+000 | | | | |
| C2H4 | 0.000e+000 | 0.000e+000 | -282.260 | -282.260 | 0.000 |
| C(-3) | 0.000e+000 | | | | |
| C2H6 | 0.000e+000 | 0.000e+000 | -254.384 | -254.384 | 0.000 |
| C(-4) | 0.000e+000 | | | | |
| CH4 | 0.000e+000 | 0.000e+000 | -156.756 | -156.756 | 0.000 |
| C(2) | 0.000e+000 | | | | |
| CO | 0.000e+000 | 0.000e+000 | -57.287 | -57.287 | 0.000 |
| C(4) | 1.369e-002 | | | | |
| CO3-2 | 1.038e-002 | 1.668e-003 | -1.984 | -2.778 | -0.794 |
| NaCO3- | 3.165e-003 | 2.092e-003 | -2.500 | -2.680 | -0.180 |
| HCO3- | 6.408e-005 | 4.234e-005 | -4.193 | -4.373 | -0.180 |
| MgCO3 | 4.928e-005 | 4.928e-005 | -4.307 | -4.307 | 0.000 |
| NaHCO3 | 2.088e-005 | 2.088e-005 | -4.680 | -4.680 | 0.000 |
| CaCO3 | 6.614e-006 | 6.614e-006 | -5.180 | -5.180 | 0.000 |
| MgHCO3+ | 2.198e-008 | 1.452e-008 | -7.658 | -7.838 | -0.180 |
| CaHCO3+ | 1.445e-009 | 9.547e-010 | -8.840 | -9.020 | -0.180 |

| | | | | | |
|---|---|---|---|---|---|
| CO2 | 8.385e-011 | 1.085e-010 | -10.076 | -9.965 | 0.112 |
| FeCO3+ | 1.226e-026 | 8.104e-027 | -25.911 | -26.091 | -0.180 |
| FeCO3 | 5.706e-028 | 5.706e-028 | -27.244 | -27.244 | 0.000 |
| FeHCO3+ | 1.832e-031 | 1.211e-031 | -30.737 | -30.917 | -0.180 |
| Ca | 1.565e-005 | | | | |
| Ca+2 | 8.629e-006 | 1.922e-006 | -5.064 | -5.716 | -0.652 |
| CaCO3 | 6.614e-006 | 6.614e-006 | -5.180 | -5.180 | 0.000 |
| CaOH+ | 3.984e-007 | 2.633e-007 | -6.400 | -6.580 | -0.180 |
| CaSO4 | 3.906e-009 | 3.906e-009 | -8.408 | -8.408 | 0.000 |
| CaHCO3+ | 1.445e-009 | 9.547e-010 | -8.840 | -9.020 | -0.180 |
| Fe(2) | 7.713e-025 | | | | |
| Fe(OH)3- | 7.518e-025 | 4.968e-025 | -24.124 | -24.304 | -0.180 |
| Fe(OH)2 | 1.287e-026 | 1.287e-026 | -25.890 | -25.890 | 0.000 |
| Fe(OH)4-2 | 3.451e-027 | 4.818e-028 | -26.462 | -27.317 | -0.855 |
| FeOH+ | 2.528e-027 | 1.671e-027 | -26.597 | -26.777 | -0.180 |
| FeCO3 | 5.706e-028 | 5.706e-028 | -27.244 | -27.244 | 0.000 |
| Fe+2 | 2.446e-029 | 5.447e-030 | -28.612 | -29.264 | -0.652 |
| FeHCO3+ | 1.832e-031 | 1.211e-031 | -30.737 | -30.917 | -0.180 |
| FeSO4 | 1.256e-032 | 1.256e-032 | -31.901 | -31.901 | 0.000 |
| Fe(3) | 1.818e-007 | | | | |
| Fe(OH)4- | 1.813e-007 | 1.198e-007 | -6.742 | -6.922 | -0.180 |
| Fe(OH)3 | 4.918e-010 | 4.918e-010 | -9.308 | -9.308 | 0.000 |
| Fe(OH)2+ | 1.641e-015 | 1.084e-015 | -14.785 | -14.965 | -0.180 |
| FeOH+2 | 2.101e-023 | 3.376e-024 | -22.678 | -23.472 | -0.794 |
| FeCO3+ | 1.226e-026 | 8.104e-027 | -25.911 | -26.091 | -0.180 |
| Fe+3 | 7.234e-033 | 5.392e-034 | -32.141 | -33.268 | -1.128 |
| FeSO4+ | 9.487e-037 | 6.269e-037 | -36.023 | -36.203 | -0.180 |
| Fe(SO4)2- | 2.824e-040 | 1.866e-040 | -39.549 | -39.729 | -0.180 |
| Fe2(OH)2+4 | 0.000e+000 | 0.000e+000 | -42.602 | -45.513 | -2.911 |
| Fe3(OH)4+5 | 0.000e+000 | 0.000e+000 | -53.845 | -58.158 | -4.313 |
| H(0) | 0.000e+000 | | | | |
| H2 | 0.000e+000 | 0.000e+000 | -45.467 | -45.355 | 0.112 |
| K | 3.932e-004 | | | | |
| K+ | 3.923e-004 | 2.374e-004 | -3.406 | -3.625 | -0.218 |
| KOH | 7.983e-007 | 7.983e-007 | -6.098 | -6.098 | 0.000 |
| KSO4- | 4.126e-008 | 2.727e-008 | -7.384 | -7.564 | -0.180 |
| KHSO4 | 2.035e-020 | 2.035e-020 | -19.691 | -19.691 | 0.000 |
| Li | 4.997e-014 | | | | |
| Li+ | 4.915e-014 | 3.650e-014 | -13.308 | -13.438 | -0.129 |
| LiOH | 8.110e-016 | 8.110e-016 | -15.091 | -15.091 | 0.000 |
| LiSO4- | 4.731e-018 | 3.127e-018 | -17.325 | -17.505 | -0.180 |
| Mg | 1.499e-004 | | | | |
| Mg+2 | 1.001e-004 | 2.995e-005 | -4.000 | -4.524 | -0.524 |
| MgCO3 | 4.928e-005 | 4.928e-005 | -4.307 | -4.307 | 0.000 |
| Mg4(OH)4+4 | 1.031e-007 | 1.266e-010 | -6.987 | -9.897 | -2.911 |
| MgSO4 | 1.020e-007 | 1.020e-007 | -6.991 | -6.991 | 0.000 |
| MgHCO3+ | 2.198e-008 | 1.452e-008 | -7.658 | -7.838 | -0.180 |
| Na | 5.907e-001 | | | | |
| Na+ | 4.747e-001 | 3.137e-001 | -0.324 | -0.504 | -0.180 |
| NaHSiO3 | 1.125e-001 | 1.125e-001 | -0.949 | -0.949 | 0.000 |
| NaCO3- | 3.165e-003 | 2.092e-003 | -2.500 | -2.680 | -0.180 |
| NaOH | 3.484e-004 | 3.484e-004 | -3.458 | -3.458 | 0.000 |
| NaSO4- | 4.562e-005 | 3.015e-005 | -4.341 | -4.521 | -0.180 |
| NaHCO3 | 2.088e-005 | 2.088e-005 | -4.680 | -4.680 | 0.000 |
| NaAlO2 | 1.039e-009 | 1.039e-009 | -8.983 | -8.983 | 0.000 |
| O(0) | 1.113e-003 | | | | |
| O2 | 5.567e-004 | 7.201e-004 | -3.254 | -3.143 | 0.112 |
| S(-2) | 0.000e+000 | | | | |
| HS- | 0.000e+000 | 0.000e+000 | -151.222 | -151.419 | -0.198 |
| S-2 | 0.000e+000 | 0.000e+000 | -151.760 | -152.501 | -0.741 |
| H2S | 0.000e+000 | 0.000e+000 | -156.334 | -156.334 | 0.000 |
| S2-2 | 0.000e+000 | 0.000e+000 | -269.643 | -270.498 | -0.855 |

```
  S3-2              0.000e+000  0.000e+000  -387.679  -388.534    -0.855
  S4-2              0.000e+000  0.000e+000  -505.945  -506.800    -0.855
  S5-2              0.000e+000  0.000e+000  -624.432  -625.287    -0.855
S(2)          0.000e+000
  S2O3-2            0.000e+000  0.000e+000  -162.545  -163.400    -0.855
  HS2O3-            0.000e+000  0.000e+000  -174.199  -174.379    -0.180
S(3)          0.000e+000
  S2O4-2            0.000e+000  0.000e+000  -148.824  -149.564    -0.741
S(4)          0.000e+000
  SO3-2             0.000e+000  0.000e+000   -49.890   -50.684    -0.794
  HSO3-             0.000e+000  0.000e+000   -55.293   -55.472    -0.180
  H2SO3             0.000e+000  0.000e+000   -65.455   -65.455     0.000
  SO2               0.000e+000  0.000e+000   -65.628   -65.628     0.000
  S2O6-2            0.000e+000  0.000e+000   -83.662   -84.517    -0.855
  S3O6-2            0.000e+000  0.000e+000  -204.204  -205.059    -0.855
  S4O6-2            0.000e+000  0.000e+000  -308.663  -309.518    -0.855
  S5O6-2            0.000e+000  0.000e+000  -442.309  -443.164    -0.855
S(5)          0.000e+000
  S2O5-2            0.000e+000  0.000e+000  -114.904  -115.759    -0.855
S(6)          1.499e-004
  SO4-2             1.042e-004  1.455e-005    -3.982    -4.837    -0.855
  NaSO4-            4.562e-005  3.015e-005    -4.341    -4.521    -0.180
  MgSO4             1.020e-007  1.020e-007    -6.991    -6.991     0.000
  KSO4-             4.126e-008  2.727e-008    -7.384    -7.564    -0.180
  CaSO4             3.906e-009  3.906e-009    -8.408    -8.408     0.000
  HSO4-             1.966e-015  1.299e-015   -14.706   -14.886    -0.180
  LiSO4-            4.731e-018  3.127e-018   -17.325   -17.505    -0.180
  KHSO4             2.035e-020  2.035e-020   -19.691   -19.691     0.000
  H2SO4             1.437e-030  1.437e-030   -29.842   -29.842     0.000
  FeSO4             1.256e-032  1.256e-032   -31.901   -31.901     0.000
  AlSO4+            1.233e-034  8.150e-035   -33.909   -34.089    -0.180
  FeSO4+            9.487e-037  6.269e-037   -36.023   -36.203    -0.180
  Al(SO4)2-         1.393e-037  9.203e-038   -36.856   -37.036    -0.180
  Fe(SO4)2-         2.824e-040  1.866e-040   -39.549   -39.729    -0.180
S(7)          0.000e+000
  S2O8-2            0.000e+000  0.000e+000   -57.407   -58.262    -0.855
S(8)          1.259e-036
  HSO5-             1.259e-036  8.320e-037   -35.900   -36.080    -0.180
Si            5.481e-001
  NaHSiO3           1.125e-001  1.125e-001    -0.949    -0.949     0.000
  H4(H2SiO4)4-4     1.049e-001  2.920e-005    -0.979    -4.535    -3.555
  HSiO3-            1.046e-002  6.916e-003    -1.980    -2.160    -0.180
  H2SiO4-2          5.476e-003  7.647e-004    -2.262    -3.117    -0.855
  SiO2              7.415e-005  7.415e-005    -4.130    -4.130     0.000
  H6(H2SiO4)4-2     4.326e-006  6.041e-007    -5.364    -6.219    -0.855
```

## File 22. Fresh Cement, Maximum ions, 50%/50% Mixing Ratio

*INPUT FILE*

```
SOLUTION 1
    temp      15
    pH        7.5 charge
    pe        4
    redox     pe
    units     mmol/kgw
    density   1
    Alkalinity 0
    Cl(-1)    7.5
    Li        1e-010
    Al        1e-010
    Ca        3.1
```

```
    Mg       5
    Na       18
    K        1.9
    S(6)     7.3
    N(5)     7.9
    C(4)     21.8
    Br(-1)   0
    Si       0.01
    -water   0.144 # kg

EQUILIBRIUM_PHASES 1
    Brucite   0 0.208
    Ca(OH)2*(CSH(1.5)) 0 1.42
    Calcite   0 0.001
    CSH(1.0-2.5) 0 2.386
    Ettringite 0 0.016
    Gibbsite  0 0.001
    Goethite  0 0.001
    Hydrogarnet(C3AH6) 0 0.384
    SiO2(am)  0 0.02
    KOH(cement) 0 0.148
    NaOH(cement) 0 0.022
    Monosulfate 0 0.192
GAS_PHASE 1
    -fixed_pressure
    -pressure 1
    -volume 1
    -temperature 25
    CO2(g)    0.056
SAVE solution 1-1
END
SOLUTION 2
    temp      25
    pH        7.5 charge
    pe        4
    redox     pe
    units     mmol/kgs
    density   1
    Li        0
    Alkalinity 0
    Ca        3.1
    Mg        5
    Na        18
    C(4)      21.8
    Cl        7.5
    S(6)      7.3
    N(5)      7.8
    Si        0.001
    K         1.9
    -water    0.144 # kg
GAS_PHASE 2
    -fixed_pressure
    -pressure 1
    -volume 1
    -temperature 25
    CO2(g)    0.056
    O2(g)     0.18
EQUILIBRIUM_PHASES 2
    calcite   0 1
SAVE solution 2-2
END
MIX 1
```

```
   1   0.5
   2   0.5
EQUILIBRIUM_PHASES 3
   Albite    0 0.6
   Calcite   0 0.1
   K-Feldspar 0 0.6
   Quartz    0 72
   SiO2(am)  0 17.3
```

*SAMPLE OUTPUT, FINAL TIME STEP (FILE 22)*

```
-------------------------------------------
Beginning of batch-reaction calculations.
-------------------------------------------

Reaction step 1.

Using mix 1.
Using pure phase assemblage 3.

Mixture 1.

       5.000e-001 Solution 1       Solution after simulation 1.
       5.000e-001 Solution 2       Solution after simulation 2.

--------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
Phase               SI log IAP  log KT      Initial       Final       Delta

Albite            -0.00    2.80    2.80   6.000e-001  5.258e-001 -7.421e-002
Calcite           -0.00    1.90    1.90   1.000e-001  1.005e-001  4.838e-004
K-Feldspar        -0.00   -0.32   -0.32   6.000e-001  6.742e-001  7.422e-002
Quartz             0.00   -4.13   -4.13   7.200e+001  8.922e+001  1.722e+001
SiO2(am)          -1.32   -4.13   -2.81   1.730e+001           0 -1.730e+001

-----------------------------Solution composition-----------------------------

      Elements          Molality       Moles

      Al             2.834e-008  4.084e-009
      C              1.709e-002  2.463e-003
      Ca             1.422e-005  2.049e-006
      Cl             7.506e-003  1.082e-003
      Fe             1.817e-007  2.619e-008
      K              4.060e-004  5.850e-005
      Li             4.996e-014  7.200e-015
      Mg             2.506e-003  3.611e-004
      N              7.857e-003  1.132e-003
      Na             6.093e-001  8.780e-002
      S              3.659e-003  5.273e-004
      Si             5.411e-001  7.797e-002

----------------------------Description of solution----------------------------

                                pH  =  11.989      Charge balance
                                pe  =   9.066      Adjusted to redox equilibrium
                     Activity of water  =   0.987
                        Ionic strength  =  1.131e+000
                     Mass of water (kg)  =  1.441e-001
                Total alkalinity (eq/kg)  =  5.921e-001
                     Total CO2 (mol/kg)  =  1.709e-002
```

Temperature (deg C) = 20.000
Electrical balance (eq) = 1.004e-012
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 0.00
Iterations = 42
Total H = 1.620158e+001
Total O = 8.309960e+000

----------Distribution of species----------

| Species | Molality | Log Activity | Log Molality | Log Activity | Gamma |
|---|---|---|---|---|---|
| OH- | 9.954e-003 | 6.315e-003 | -2.002 | -2.200 | -0.198 |
| H+ | 1.248e-012 | 1.026e-012 | -11.904 | -11.989 | -0.085 |
| H2O | 5.553e+001 | 9.869e-001 | 1.744 | -0.006 | 0.000 |
| Al | 2.834e-008 | | | | |
| AlO2- | 2.730e-008 | 1.804e-008 | -7.564 | -7.744 | -0.180 |
| NaAlO2 | 1.039e-009 | 1.039e-009 | -8.983 | -8.983 | 0.000 |
| HAlO2 | 6.937e-014 | 6.937e-014 | -13.159 | -13.159 | 0.000 |
| Al(OH)2+ | 1.018e-019 | 6.727e-020 | -18.992 | -19.172 | -0.180 |
| AlOH+2 | 2.626e-025 | 4.209e-026 | -24.581 | -25.376 | -0.795 |
| Al+3 | 7.388e-032 | 5.496e-033 | -31.131 | -32.260 | -1.129 |
| AlSO4+ | 2.975e-033 | 1.966e-033 | -32.527 | -32.706 | -0.180 |
| Al(SO4)2- | 8.071e-035 | 5.334e-035 | -34.093 | -34.273 | -0.180 |
| Al2(OH)2+4 | 0.000e+000 | 0.000e+000 | -45.329 | -48.244 | -2.915 |
| Al3(OH)4+5 | 0.000e+000 | 0.000e+000 | -58.409 | -62.728 | -4.319 |
| Al13O4(OH)24+7 | 0.000e+000 | 0.000e+000 | -126.122 | -134.632 | -8.510 |
| C(-2) | 0.000e+000 | | | | |
| C2H4 | 0.000e+000 | 0.000e+000 | -281.836 | -281.836 | 0.000 |
| C(-3) | 0.000e+000 | | | | |
| C2H6 | 0.000e+000 | 0.000e+000 | -253.919 | -253.919 | 0.000 |
| C(-4) | 0.000e+000 | | | | |
| CH4 | 0.000e+000 | 0.000e+000 | -156.503 | -156.503 | 0.000 |
| C(2) | 0.000e+000 | | | | |
| CO | 0.000e+000 | 0.000e+000 | -57.156 | -57.156 | 0.000 |
| C(4) | 1.709e-002 | | | | |
| CO3-2 | 1.259e-002 | 2.018e-003 | -1.900 | -2.695 | -0.795 |
| NaCO3- | 3.943e-003 | 2.606e-003 | -2.404 | -2.584 | -0.180 |
| MgCO3 | 4.483e-004 | 4.483e-004 | -3.348 | -3.348 | 0.000 |
| HCO3- | 7.815e-005 | 5.164e-005 | -4.107 | -4.287 | -0.180 |
| NaHCO3 | 2.622e-005 | 2.622e-005 | -4.581 | -4.581 | 0.000 |
| CaCO3 | 6.614e-006 | 6.614e-006 | -5.180 | -5.180 | 0.000 |
| MgHCO3+ | 2.015e-007 | 1.331e-007 | -6.696 | -6.876 | -0.180 |
| CaHCO3+ | 1.456e-009 | 9.623e-010 | -8.837 | -9.017 | -0.180 |
| CO2 | 1.029e-010 | 1.334e-010 | -9.988 | -9.875 | 0.113 |
| FeCO3+ | 1.535e-026 | 1.014e-026 | -25.814 | -25.994 | -0.180 |
| FeCO3 | 7.424e-028 | 7.424e-028 | -27.129 | -27.129 | 0.000 |
| FeHCO3+ | 2.402e-031 | 1.588e-031 | -30.619 | -30.799 | -0.180 |
| Ca | 1.422e-005 | | | | |
| Ca+2 | 7.142e-006 | 1.588e-006 | -5.146 | -5.799 | -0.653 |
| CaCO3 | 6.614e-006 | 6.614e-006 | -5.180 | -5.180 | 0.000 |
| CaOH+ | 3.265e-007 | 2.157e-007 | -6.486 | -6.666 | -0.180 |
| CaSO4 | 7.757e-008 | 7.757e-008 | -7.110 | -7.110 | 0.000 |
| CaNO3+ | 5.725e-008 | 3.783e-008 | -7.242 | -7.422 | -0.180 |
| CaCl+ | 2.205e-009 | 1.457e-009 | -8.656 | -8.836 | -0.180 |
| CaHCO3+ | 1.456e-009 | 9.623e-010 | -8.837 | -9.017 | -0.180 |
| CaCl2 | 7.935e-012 | 7.935e-012 | -11.100 | -11.100 | 0.000 |
| Cl(-1) | 7.506e-003 | | | | |
| Cl- | 7.265e-003 | 4.394e-003 | -2.139 | -2.357 | -0.218 |
| NaCl | 2.402e-004 | 2.402e-004 | -3.619 | -3.619 | 0.000 |
| MgCl+ | 1.174e-006 | 7.757e-007 | -5.930 | -6.110 | -0.180 |
| KCl | 3.259e-008 | 3.259e-008 | -7.487 | -7.487 | 0.000 |

| | | | | | |
|---|---|---|---|---|---|
| CaCl+ | 2.205e-009 | 1.457e-009 | -8.656 | -8.836 | -0.180 |
| CaCl2 | 7.935e-012 | 7.935e-012 | -11.100 | -11.100 | 0.000 |
| HCl | 1.006e-015 | 1.006e-015 | -14.997 | -14.997 | 0.000 |
| LiCl | 5.069e-018 | 5.069e-018 | -17.295 | -17.295 | 0.000 |
| FeCl+ | 2.777e-032 | 1.835e-032 | -31.556 | -31.736 | -0.180 |
| FeCl2+ | 2.199e-036 | 1.453e-036 | -35.658 | -35.838 | -0.180 |
| FeCl+2 | 1.975e-036 | 3.166e-037 | -35.704 | -36.499 | -0.795 |
| FeCl2 | 4.216e-037 | 4.216e-037 | -36.375 | -36.375 | 0.000 |
| FeCl4-2 | 1.665e-040 | 0.000e+000 | -39.778 | -40.635 | -0.856 |
| FeCl4- | 0.000e+000 | 0.000e+000 | -43.292 | -43.472 | -0.180 |
| Cl(1) | 7.995e-020 | | | | |
| ClO- | 7.995e-020 | 5.283e-020 | -19.097 | -19.277 | -0.180 |
| HClO | 2.011e-024 | 2.011e-024 | -23.697 | -23.697 | 0.000 |
| Cl(3) | 1.392e-029 | | | | |
| ClO2- | 1.392e-029 | 9.200e-030 | -28.856 | -29.036 | -0.180 |
| HClO2 | 1.396e-038 | 1.396e-038 | -37.855 | -37.855 | 0.000 |
| Cl(5) | 3.087e-025 | | | | |
| ClO3- | 3.087e-025 | 1.958e-025 | -24.511 | -24.708 | -0.198 |
| Cl(7) | 3.012e-025 | | | | |
| ClO4- | 3.012e-025 | 1.911e-025 | -24.521 | -24.719 | -0.198 |
| Fe(2) | 8.088e-025 | | | | |
| Fe(OH)3- | 7.881e-025 | 5.208e-025 | -24.103 | -24.283 | -0.180 |
| Fe(OH)2 | 1.360e-026 | 1.360e-026 | -25.866 | -25.866 | 0.000 |
| Fe(OH)4-2 | 3.597e-027 | 5.008e-028 | -26.444 | -27.300 | -0.856 |
| FeOH+ | 2.695e-027 | 1.781e-027 | -26.569 | -26.749 | -0.180 |
| FeCO3 | 7.424e-028 | 7.424e-028 | -27.129 | -27.129 | 0.000 |
| Fe+2 | 2.634e-029 | 5.858e-030 | -28.579 | -29.232 | -0.653 |
| FeSO4 | 3.245e-031 | 3.245e-031 | -30.489 | -30.489 | 0.000 |
| FeHCO3+ | 2.402e-031 | 1.588e-031 | -30.619 | -30.799 | -0.180 |
| FeCl+ | 2.777e-032 | 1.835e-032 | -31.556 | -31.736 | -0.180 |
| FeCl2 | 4.216e-037 | 4.216e-037 | -36.375 | -36.375 | 0.000 |
| FeCl4-2 | 1.665e-040 | 0.000e+000 | -39.778 | -40.635 | -0.856 |
| Fe(3) | 1.817e-007 | | | | |
| Fe(OH)4- | 1.812e-007 | 1.198e-007 | -6.742 | -6.922 | -0.180 |
| Fe(OH)3 | 4.959e-010 | 4.959e-010 | -9.305 | -9.305 | 0.000 |
| Fe(OH)2+ | 1.668e-015 | 1.103e-015 | -14.778 | -14.958 | -0.180 |
| FeOH+2 | 2.160e-023 | 3.463e-024 | -22.666 | -23.461 | -0.795 |
| FeCO3+ | 1.535e-026 | 1.014e-026 | -25.814 | -25.994 | -0.180 |
| Fe+3 | 7.499e-033 | 5.578e-034 | -32.125 | -33.254 | -1.129 |
| FeNO3+2 | 1.653e-034 | 2.651e-035 | -33.782 | -34.577 | -0.795 |
| FeSO4+ | 2.358e-035 | 1.559e-035 | -34.627 | -34.807 | -0.180 |
| FeCl2+ | 2.199e-036 | 1.453e-036 | -35.658 | -35.838 | -0.180 |
| FeCl+2 | 1.975e-036 | 3.166e-037 | -35.704 | -36.499 | -0.795 |
| Fe(SO4)2- | 1.687e-037 | 1.115e-037 | -36.773 | -36.953 | -0.180 |
| Fe2(OH)2+4 | 0.000e+000 | 0.000e+000 | -42.576 | -45.491 | -2.915 |
| FeCl4- | 0.000e+000 | 0.000e+000 | -43.292 | -43.472 | -0.180 |
| FeNO2+2 | 0.000e+000 | 0.000e+000 | -45.539 | -46.334 | -0.795 |
| Fe3(OH)4+5 | 0.000e+000 | 0.000e+000 | -53.809 | -58.129 | -4.319 |
| H(0) | 0.000e+000 | | | | |
| H2 | 0.000e+000 | 0.000e+000 | -45.427 | -45.314 | 0.113 |
| K | 4.060e-004 | | | | |
| K+ | 4.041e-004 | 2.444e-004 | -3.393 | -3.612 | -0.218 |
| KSO4- | 1.021e-006 | 6.747e-007 | -5.991 | -6.171 | -0.180 |
| KOH | 8.150e-007 | 8.150e-007 | -6.089 | -6.089 | 0.000 |
| KCl | 3.259e-008 | 3.259e-008 | -7.487 | -7.487 | 0.000 |
| KHSO4 | 5.075e-019 | 5.075e-019 | -18.295 | -18.295 | 0.000 |
| Li | 4.996e-014 | | | | |
| Li+ | 4.904e-014 | 3.644e-014 | -13.309 | -13.438 | -0.129 |
| LiOH | 8.026e-016 | 8.026e-016 | -15.096 | -15.096 | 0.000 |
| LiSO4- | 1.135e-016 | 7.500e-017 | -15.945 | -16.125 | -0.180 |
| LiCl | 5.069e-018 | 5.069e-018 | -17.295 | -17.295 | 0.000 |
| Mg | 2.506e-003 | | | | |

| | | | | | |
|---|---|---|---|---|---|
| Mg+2 | 7.530e-004 | 2.252e-004 | -3.123 | -3.647 | -0.524 |
| MgCO3 | 4.483e-004 | 4.483e-004 | -3.348 | -3.348 | 0.000 |
| Mg4(OH)4+4 | 3.212e-004 | 3.908e-007 | -3.493 | -6.408 | -2.915 |
| MgSO4 | 1.843e-005 | 1.843e-005 | -4.735 | -4.735 | 0.000 |
| MgCl+ | 1.174e-006 | 7.757e-007 | -5.930 | -6.110 | -0.180 |
| MgHCO3+ | 2.015e-007 | 1.331e-007 | -6.696 | -6.876 | -0.180 |
| N(-03) | 0.000e+000 | | | | |
| N3- | 0.000e+000 | 0.000e+000 | -108.797 | -108.977 | -0.180 |
| HN3 | 0.000e+000 | 0.000e+000 | -116.218 | -116.218 | 0.000 |
| N(-3) | 0.000e+000 | | | | |
| NH3 | 0.000e+000 | 0.000e+000 | -71.091 | -71.091 | 0.000 |
| NH4+ | 0.000e+000 | 0.000e+000 | -73.442 | -73.685 | -0.243 |
| NH4SO4- | 0.000e+000 | 0.000e+000 | -85.417 | -85.596 | -0.180 |
| N(0) | 6.446e-029 | | | | |
| N2 | 3.223e-029 | 3.223e-029 | -28.492 | -28.492 | 0.000 |
| N(3) | 9.731e-017 | | | | |
| NO2- | 9.731e-017 | 5.886e-017 | -16.012 | -16.230 | -0.218 |
| HNO2 | 1.144e-025 | 1.144e-025 | -24.941 | -24.941 | 0.000 |
| FeNO2+2 | 0.000e+000 | 0.000e+000 | -45.539 | -46.334 | -0.795 |
| N(5) | 7.857e-003 | | | | |
| NO3- | 7.857e-003 | 4.752e-003 | -2.105 | -2.323 | -0.218 |
| CaNO3+ | 5.725e-008 | 3.783e-008 | -7.242 | -7.422 | -0.180 |
| HNO3 | 2.265e-016 | 2.265e-016 | -15.645 | -15.645 | 0.000 |
| FeNO3+2 | 1.653e-034 | 2.651e-035 | -33.782 | -34.577 | -0.795 |
| Na | 6.093e-001 | | | | |
| Na+ | 4.888e-001 | 3.230e-001 | -0.311 | -0.491 | -0.180 |
| NaHSiO3 | 1.149e-001 | 1.149e-001 | -0.940 | -0.940 | 0.000 |
| NaCO3- | 3.943e-003 | 2.606e-003 | -2.404 | -2.584 | -0.180 |
| NaSO4- | 1.129e-003 | 7.459e-004 | -2.947 | -3.127 | -0.180 |
| NaOH | 3.557e-004 | 3.557e-004 | -3.449 | -3.449 | 0.000 |
| NaCl | 2.402e-004 | 2.402e-004 | -3.619 | -3.619 | 0.000 |
| NaHCO3 | 2.622e-005 | 2.622e-005 | -4.581 | -4.581 | 0.000 |
| NaAlO2 | 1.039e-009 | 1.039e-009 | -8.983 | -8.983 | 0.000 |
| O(0) | 9.206e-004 | | | | |
| O2 | 4.603e-004 | 5.966e-004 | -3.337 | -3.224 | 0.113 |
| S(-2) | 0.000e+000 | | | | |
| HS- | 0.000e+000 | 0.000e+000 | -149.674 | -149.872 | -0.198 |
| S-2 | 0.000e+000 | 0.000e+000 | -150.215 | -150.957 | -0.742 |
| H2S | 0.000e+000 | 0.000e+000 | -154.783 | -154.783 | 0.000 |
| S2-2 | 0.000e+000 | 0.000e+000 | -266.587 | -267.443 | -0.856 |
| S3-2 | 0.000e+000 | 0.000e+000 | -383.113 | -383.969 | -0.856 |
| S4-2 | 0.000e+000 | 0.000e+000 | -499.868 | -500.725 | -0.856 |
| S5-2 | 0.000e+000 | 0.000e+000 | -616.845 | -617.701 | -0.856 |
| S(2) | 0.000e+000 | | | | |
| S2O3-2 | 0.000e+000 | 0.000e+000 | -159.612 | -160.468 | -0.856 |
| HS2O3- | 0.000e+000 | 0.000e+000 | -171.263 | -171.443 | -0.180 |
| S(3) | 0.000e+000 | | | | |
| S2O4-2 | 0.000e+000 | 0.000e+000 | -145.932 | -146.673 | -0.742 |
| S(4) | 0.000e+000 | | | | |
| SO3-2 | 0.000e+000 | 0.000e+000 | -48.468 | -49.263 | -0.795 |
| HSO3- | 0.000e+000 | 0.000e+000 | -53.867 | -54.047 | -0.180 |
| H2SO3 | 0.000e+000 | 0.000e+000 | -64.027 | -64.027 | 0.000 |
| SO2 | 0.000e+000 | 0.000e+000 | -64.199 | -64.199 | 0.000 |
| S2O6-2 | 0.000e+000 | 0.000e+000 | -80.851 | -81.707 | -0.856 |
| S3O6-2 | 0.000e+000 | 0.000e+000 | -199.882 | -200.739 | -0.856 |
| S4O6-2 | 0.000e+000 | 0.000e+000 | -302.832 | -303.688 | -0.856 |
| S5O6-2 | 0.000e+000 | 0.000e+000 | -434.967 | -435.823 | -0.856 |
| S(5) | 0.000e+000 | | | | |
| S2O5-2 | 0.000e+000 | 0.000e+000 | -112.052 | -112.908 | -0.856 |
| S(6) | 3.659e-003 | | | | |
| SO4-2 | 2.511e-003 | 3.496e-004 | -2.600 | -3.456 | -0.856 |
| NaSO4- | 1.129e-003 | 7.459e-004 | -2.947 | -3.127 | -0.180 |

```
   MgSO4              1.843e-005  1.843e-005    -4.735    -4.735     0.000
   KSO4-              1.021e-006  6.747e-007    -5.991    -6.171    -0.180
   CaSO4              7.757e-008  7.757e-008    -7.110    -7.110     0.000
   HSO4-              4.762e-014  3.147e-014   -13.322   -13.502    -0.180
   LiSO4-             1.135e-016  7.500e-017   -15.945   -16.125    -0.180
   KHSO4              5.075e-019  5.075e-019   -18.295   -18.295     0.000
   H2SO4              3.509e-029  3.509e-029   -28.455   -28.455     0.000
   FeSO4              3.245e-031  3.245e-031   -30.489   -30.489     0.000
   AlSO4+             2.975e-033  1.966e-033   -32.527   -32.706    -0.180
   Al(SO4)2-          8.071e-035  5.334e-035   -34.093   -34.273    -0.180
   FeSO4+             2.358e-035  1.559e-035   -34.627   -34.807    -0.180
   Fe(SO4)2-          1.687e-037  1.115e-037   -36.773   -36.953    -0.180
   NH4SO4-            0.000e+000  0.000e+000   -85.417   -85.596    -0.180
S(7)          0.000e+000
   S2O8-2             0.000e+000  0.000e+000   -54.678   -55.534    -0.856
S(8)          2.776e-035
   HSO5-              2.776e-035  1.834e-035   -34.557   -34.736    -0.180
Si            5.411e-001
   NaHSiO3            1.149e-001  1.149e-001    -0.940    -0.940     0.000
   H4(H2SiO4)4-4      1.026e-001  2.815e-005    -0.989    -4.551    -3.562
   HSiO3-             1.038e-002  6.857e-003    -1.984    -2.164    -0.180
   H2SiO4-2           5.399e-003  7.517e-004    -2.268    -3.124    -0.856
   SiO2               7.415e-005  7.415e-005    -4.130    -4.130     0.000
   H6(H2SiO4)4-2      4.249e-006  5.916e-007    -5.372    -6.228    -0.856
```

## File 23. Mature Cement, Minimum ions, 95%/5% Mixing Ratio

*INPUT FILE*

```
SOLUTION 1
    temp      15
    pH        7.5 charge
    pe        4
    redox     pe
    units     mmol/kgw
    density   1
    Alkalinity 0
    Cl(-1)    0.001
    Li        1e-010
    Al        1e-010
    Ca        0.6
    Mg        0.3
    Na        1.3
    K         0
    S(6)      0.3
    N(5)      0
    C(4)      1.4
    Br(-1)    0
    Si        0.01
    -water    0.144 # kg

EQUILIBRIUM_PHASES 1
    Brucite   0 0.208
    Ca(OH)2*(CSH(1.5)) 0 1.42
    Calcite   0 0.001
    CSH(1.0-2.5) 0 2.386
    Ettringite 0 0.016
    Gibbsite  0 0.001
    Goethite  0 0.001
    Hydrogarnet(C3AH6) 0 0.384
    SiO2(am)  0 0.02
GAS_PHASE 1
```

```
    -fixed_pressure
    -pressure 1
    -volume 1
    -temperature 25
    CO2(g)    0.056
SAVE solution 1-1
END
SOLUTION 2
    temp      25
    pH        7.5 charge
    pe        4
    redox     pe
    units     mmol/kgw
    density   1
    Li        0
    Alkalinity 0
    Ca        0.6
    Mg        0.3
    Na        1.3
    C(4)      1.4
    Cl        0.001
    S(6)      0.3
    N(5)      0
    Si        0.001
    K         0
    -water    0.144 # kg
GAS_PHASE 2
    -fixed_pressure
    -pressure 1
    -volume 1
    -temperature 25
    CO2(g)    0.056
    O2(g)     0.18
EQUILIBRIUM_PHASES 2
    calcite   0 1
SAVE solution 2-2
END
MIX 1
    1    0.95
    2    0.05
EQUILIBRIUM_PHASES 3
    Albite    0 0.6
    calcite   0 0.1
    K-Feldspar 0 0.6
    Quartz    0 72
    SiO2(am)  0 17.3
```

*SAMPLE OUTPUT, FINAL TIME STEP (FILE 23)*

```
------------------------------------------
Beginning of batch-reaction calculations.
------------------------------------------

Reaction step 1.

Using mix 1.
Using pure phase assemblage 3.

Mixture 1.

        9.500e-001 Solution 1       Solution after simulation 1.
        5.000e-002 Solution 2       Solution after simulation 2.
```

----------Phase assemblage----------

| Phase | SI | log IAP | log KT | Moles in assemblage Initial | Final | Delta |
|---|---|---|---|---|---|---|
| Albite | -0.00 | 2.93 | 2.93 | 6.000e-001 | 6.000e-001 | -7.115e-007 |
| Calcite | -0.00 | 1.97 | 1.97 | 1.000e-001 | 1.001e-001 | 9.427e-005 |
| K-Feldspar | -0.00 | -0.27 | -0.27 | 6.000e-001 | 6.000e-001 | -1.067e-007 |
| Quartz | 0.00 | -4.23 | -4.23 | 7.200e+001 | 8.930e+001 | 1.730e+001 |
| SiO2(am) | -1.36 | -4.23 | -2.87 | 1.730e+001 | 0 | -1.730e+001 |

----------Solution composition----------

| Elements | Molality | Moles |
|---|---|---|
| Al | 6.609e-006 | 9.543e-007 |
| C | 7.510e-006 | 1.084e-006 |
| Ca | 2.030e-002 | 2.932e-003 |
| Cl | 9.972e-007 | 1.440e-007 |
| Fe | 3.912e-009 | 5.649e-010 |
| K | 7.392e-007 | 1.067e-007 |
| Li | 9.474e-014 | 1.368e-014 |
| Mg | 1.506e-005 | 2.174e-006 |
| Na | 1.301e-003 | 1.879e-004 |
| S | 1.616e-002 | 2.334e-003 |
| Si | 4.777e-003 | 6.898e-004 |

----------Description of solution----------

pH = 11.793 Charge balance
pe = 9.337 Adjusted to redox equilibrium
Activity of water = 0.999
Ionic strength = 5.921e-002
Mass of water (kg) = 1.444e-001
Total alkalinity (eq/kg) = 9.631e-003
Total CO2 (mol/kg) = 7.510e-006
Temperature (deg C) = 15.500
Electrical balance (eq) = -1.398e-013
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.00
Iterations = 19
Total H = 1.603699e+001
Total O = 8.029924e+000

----------Distribution of species----------

| Species | Molality | Log Activity | Log Molality | Log Activity | Gamma |
|---|---|---|---|---|---|
| OH- | 3.530e-003 | 2.845e-003 | -2.452 | -2.546 | -0.094 |
| H+ | 1.888e-012 | 1.610e-012 | -11.724 | -11.793 | -0.069 |
| H2O | 5.553e+001 | 9.993e-001 | 1.744 | -0.000 | 0.000 |
| Al | 6.609e-006 | | | | |
| AlO2- | 6.608e-006 | 5.361e-006 | -5.180 | -5.271 | -0.091 |
| NaAlO2 | 8.106e-010 | 8.106e-010 | -9.091 | -9.091 | 0.000 |
| HAlO2 | 4.093e-011 | 4.093e-011 | -10.388 | -10.388 | 0.000 |
| Al(OH)2+ | 1.031e-016 | 8.367e-017 | -15.987 | -16.077 | -0.091 |
| AlOH+2 | 2.532e-022 | 1.107e-022 | -21.597 | -21.956 | -0.359 |
| AlSO4+ | 1.899e-028 | 1.541e-028 | -27.721 | -27.812 | -0.091 |
| Al+3 | 1.342e-028 | 3.065e-029 | -27.872 | -28.514 | -0.641 |
| Al(SO4)2- | 7.242e-029 | 5.876e-029 | -28.140 | -28.231 | -0.091 |
| Al2(OH)2+4 | 1.708e-040 | 0.000e+000 | -39.767 | -41.131 | -1.364 |

| | | | | | |
|---|---|---|---|---|---|
| Al3(OH)4+5 | 0.000e+000 | 0.000e+000 | -50.174 | -52.249 | -2.075 |
| Al13O4(OH)24+7 | 0.000e+000 | 0.000e+000 | -87.962 | -92.031 | -4.069 |
| C(-2) | 0.000e+000 | | | | |
| C2H4 | 0.000e+000 | 0.000e+000 | -289.333 | -289.333 | 0.000 |
| C(-3) | 0.000e+000 | | | | |
| C2H6 | 0.000e+000 | 0.000e+000 | -260.509 | -260.509 | 0.000 |
| C(-4) | 0.000e+000 | | | | |
| CH4 | 0.000e+000 | 0.000e+000 | -160.019 | -160.019 | 0.000 |
| C(2) | 0.000e+000 | | | | |
| CO | 0.000e+000 | 0.000e+000 | -60.592 | -60.592 | 0.000 |
| C(4) | 7.510e-006 | | | | |
| CaCO3 | 6.353e-006 | 6.353e-006 | -5.197 | -5.197 | 0.000 |
| CO3-2 | 1.123e-006 | 4.910e-007 | -5.950 | -6.309 | -0.359 |
| HCO3- | 2.678e-008 | 2.173e-008 | -7.572 | -7.663 | -0.091 |
| NaCO3- | 2.439e-009 | 1.979e-009 | -8.613 | -8.704 | -0.091 |
| MgCO3 | 2.272e-009 | 2.272e-009 | -8.644 | -8.644 | 0.000 |
| CaHCO3+ | 2.187e-009 | 1.774e-009 | -8.660 | -8.751 | -0.091 |
| NaHCO3 | 3.357e-011 | 3.357e-011 | -10.474 | -10.474 | 0.000 |
| MgHCO3+ | 1.524e-012 | 1.237e-012 | -11.817 | -11.908 | -0.091 |
| CO2 | 9.203e-014 | 9.336e-014 | -13.036 | -13.030 | 0.006 |
| FeCO3+ | 7.062e-031 | 5.730e-031 | -30.151 | -30.242 | -0.091 |
| FeCO3 | 1.885e-032 | 1.885e-032 | -31.725 | -31.725 | 0.000 |
| FeHCO3+ | 7.792e-036 | 6.322e-036 | -35.108 | -35.199 | -0.091 |
| Ca | 2.030e-002 | | | | |
| Ca+2 | 1.494e-002 | 6.988e-003 | -1.826 | -2.156 | -0.330 |
| CaSO4 | 4.600e-003 | 4.600e-003 | -2.337 | -2.337 | 0.000 |
| CaOH+ | 7.552e-004 | 6.128e-004 | -3.122 | -3.213 | -0.091 |
| CaCO3 | 6.353e-006 | 6.353e-006 | -5.197 | -5.197 | 0.000 |
| CaHCO3+ | 2.187e-009 | 1.774e-009 | -8.660 | -8.751 | -0.091 |
| CaCl+ | 1.419e-009 | 1.151e-009 | -8.848 | -8.939 | -0.091 |
| CaCl2 | 1.195e-015 | 1.195e-015 | -14.922 | -14.922 | 0.000 |
| Cl(-1) | 9.972e-007 | | | | |
| Cl- | 9.957e-007 | 7.968e-007 | -6.002 | -6.099 | -0.097 |
| CaCl+ | 1.419e-009 | 1.151e-009 | -8.848 | -8.939 | -0.091 |
| NaCl | 1.174e-010 | 1.174e-010 | -9.930 | -9.930 | 0.000 |
| MgCl+ | 3.893e-012 | 3.159e-012 | -11.410 | -11.500 | -0.091 |
| KCl | 1.251e-014 | 1.251e-014 | -13.903 | -13.903 | 0.000 |
| CaCl2 | 1.195e-015 | 1.195e-015 | -14.922 | -14.922 | 0.000 |
| HCl | 2.831e-019 | 2.831e-019 | -18.548 | -18.548 | 0.000 |
| LiCl | 1.845e-021 | 1.845e-021 | -20.734 | -20.734 | 0.000 |
| FeCl+ | 3.818e-037 | 3.098e-037 | -36.418 | -36.509 | -0.091 |
| FeCl+2 | 0.000e+000 | 0.000e+000 | -40.802 | -41.161 | -0.359 |
| FeCl2+ | 0.000e+000 | 0.000e+000 | -44.049 | -44.140 | -0.091 |
| FeCl2 | 0.000e+000 | 0.000e+000 | -44.899 | -44.899 | 0.000 |
| FeCl4-2 | 0.000e+000 | 0.000e+000 | -56.271 | -56.642 | -0.370 |
| FeCl4- | 0.000e+000 | 0.000e+000 | -59.166 | -59.257 | -0.091 |
| Cl(1) | 2.370e-024 | | | | |
| ClO- | 2.370e-024 | 1.923e-024 | -23.625 | -23.716 | -0.091 |
| HClO | 1.148e-028 | 1.148e-028 | -27.940 | -27.940 | 0.000 |
| Cl(3) | 9.357e-035 | | | | |
| ClO2- | 9.357e-035 | 7.591e-035 | -34.029 | -34.120 | -0.091 |
| HClO2 | 0.000e+000 | 0.000e+000 | -42.743 | -42.743 | 0.000 |
| Cl(5) | 7.520e-031 | | | | |
| ClO3- | 7.520e-031 | 6.061e-031 | -30.124 | -30.217 | -0.094 |
| Cl(7) | 2.541e-031 | | | | |
| ClO4- | 2.541e-031 | 2.048e-031 | -30.595 | -30.689 | -0.094 |
| Fe(2) | 1.704e-026 | | | | |
| Fe(OH)3- | 1.635e-026 | 1.326e-026 | -25.787 | -25.877 | -0.091 |
| Fe(OH)2 | 5.366e-028 | 5.366e-028 | -27.270 | -27.270 | 0.000 |
| FeOH+ | 1.341e-028 | 1.088e-028 | -27.872 | -27.963 | -0.091 |
| Fe(OH)4-2 | 1.931e-029 | 8.233e-030 | -28.714 | -29.084 | -0.370 |
| Fe+2 | 1.185e-030 | 5.544e-031 | -29.926 | -30.256 | -0.330 |

| | | | | | |
|---|---|---|---|---|---|
| FeSO4 | 4.316e-031 | 4.316e-031 | -30.365 | -30.365 | 0.000 |
| FeCO3 | 1.885e-032 | 1.885e-032 | -31.725 | -31.725 | 0.000 |
| FeHCO3+ | 7.792e-036 | 6.322e-036 | -35.108 | -35.199 | -0.091 |
| FeCl+ | 3.818e-037 | 3.098e-037 | -36.418 | -36.509 | -0.091 |
| FeCl2 | 0.000e+000 | 0.000e+000 | -44.899 | -44.899 | 0.000 |
| FeCl4-2 | 0.000e+000 | 0.000e+000 | -56.271 | -56.642 | -0.370 |
| Fe(3) | 3.912e-009 | | | | |
| Fe(OH)4- | 3.892e-009 | 3.158e-009 | -8.410 | -8.501 | -0.091 |
| Fe(OH)3 | 2.025e-011 | 2.025e-011 | -10.694 | -10.694 | 0.000 |
| Fe(OH)2+ | 8.596e-017 | 6.975e-017 | -16.066 | -16.156 | -0.091 |
| FeOH+2 | 7.760e-025 | 3.393e-025 | -24.110 | -24.469 | -0.359 |
| FeCO3+ | 7.062e-031 | 5.730e-031 | -30.151 | -30.242 | -0.091 |
| Fe+3 | 3.707e-034 | 8.465e-035 | -33.431 | -34.072 | -0.641 |
| FeSO4+ | 3.458e-035 | 2.806e-035 | -34.461 | -34.552 | -0.091 |
| Fe(SO4)2- | 4.119e-036 | 3.342e-036 | -35.385 | -35.476 | -0.091 |
| FeCl+2 | 0.000e+000 | 0.000e+000 | -40.802 | -41.161 | -0.359 |
| FeCl2+ | 0.000e+000 | 0.000e+000 | -44.049 | -44.140 | -0.091 |
| Fe2(OH)2+4 | 0.000e+000 | 0.000e+000 | -46.145 | -47.509 | -1.364 |
| FeCl4- | 0.000e+000 | 0.000e+000 | -59.166 | -59.257 | -0.091 |
| Fe3(OH)4+5 | 0.000e+000 | 0.000e+000 | -59.270 | -61.345 | -2.075 |
| H(0) | 0.000e+000 | | | | |
| H2 | 0.000e+000 | 0.000e+000 | -45.565 | -45.559 | 0.006 |
| K | 7.392e-007 | | | | |
| K+ | 7.113e-007 | 5.692e-007 | -6.148 | -6.245 | -0.097 |
| KSO4- | 2.673e-008 | 2.169e-008 | -7.573 | -7.664 | -0.091 |
| KOH | 1.225e-009 | 1.225e-009 | -8.912 | -8.912 | 0.000 |
| KCl | 1.251e-014 | 1.251e-014 | -13.903 | -13.903 | 0.000 |
| KHSO4 | 2.162e-020 | 2.162e-020 | -19.665 | -19.665 | 0.000 |
| Li | 9.474e-014 | | | | |
| Li+ | 9.097e-014 | 7.554e-014 | -13.041 | -13.122 | -0.081 |
| LiSO4- | 2.693e-015 | 2.185e-015 | -14.570 | -14.661 | -0.091 |
| LiOH | 1.074e-015 | 1.074e-015 | -14.969 | -14.969 | 0.000 |
| LiCl | 1.845e-021 | 1.845e-021 | -20.734 | -20.734 | 0.000 |
| Mg | 1.506e-005 | | | | |
| Mg+2 | 9.940e-006 | 5.009e-006 | -5.003 | -5.300 | -0.298 |
| MgSO4 | 5.115e-006 | 5.115e-006 | -5.291 | -5.291 | 0.000 |
| MgCO3 | 2.272e-009 | 2.272e-009 | -8.644 | -8.644 | 0.000 |
| MgCl+ | 3.893e-012 | 3.159e-012 | -11.410 | -11.500 | -0.091 |
| MgHCO3+ | 1.524e-012 | 1.237e-012 | -11.817 | -11.908 | -0.091 |
| Mg4(OH)4+4 | 3.842e-013 | 1.662e-014 | -12.415 | -13.779 | -1.364 |
| Na | 1.301e-003 | | | | |
| Na+ | 1.111e-003 | 9.011e-004 | -2.954 | -3.045 | -0.091 |
| NaHSiO3 | 1.542e-004 | 1.542e-004 | -3.812 | -3.812 | 0.000 |
| NaSO4- | 3.605e-005 | 2.925e-005 | -4.443 | -4.534 | -0.091 |
| NaOH | 4.527e-007 | 4.527e-007 | -6.344 | -6.344 | 0.000 |
| NaCO3- | 2.439e-009 | 1.979e-009 | -8.613 | -8.704 | -0.091 |
| NaAlO2 | 8.106e-010 | 8.106e-010 | -9.091 | -9.091 | 0.000 |
| NaCl | 1.174e-010 | 1.174e-010 | -9.930 | -9.930 | 0.000 |
| NaHCO3 | 3.357e-011 | 3.357e-011 | -10.474 | -10.474 | 0.000 |
| O(0) | 1.111e-004 | | | | |
| O2 | 5.556e-005 | 5.636e-005 | -4.255 | -4.249 | 0.006 |
| S(-2) | 0.000e+000 | | | | |
| HS- | 0.000e+000 | 0.000e+000 | -148.789 | -148.882 | -0.094 |
| S-2 | 0.000e+000 | 0.000e+000 | -149.951 | -150.300 | -0.349 |
| H2S | 0.000e+000 | 0.000e+000 | -153.532 | -153.532 | 0.000 |
| S2-2 | 0.000e+000 | 0.000e+000 | -265.010 | -265.380 | -0.370 |
| S3-2 | 0.000e+000 | 0.000e+000 | -380.127 | -380.497 | -0.370 |
| S4-2 | 0.000e+000 | 0.000e+000 | -495.475 | -495.845 | -0.370 |
| S5-2 | 0.000e+000 | 0.000e+000 | -611.048 | -611.418 | -0.370 |
| S(2) | 0.000e+000 | | | | |
| S2O3-2 | 0.000e+000 | 0.000e+000 | -157.739 | -158.109 | -0.370 |
| HS2O3- | 0.000e+000 | 0.000e+000 | -168.798 | -168.889 | -0.091 |

```
S(3)          0.000e+000
  S2O4-2            0.000e+000  0.000e+000  -144.162  -144.511    -0.349
S(4)          0.000e+000
  SO3-2             0.000e+000  0.000e+000   -47.987   -48.346    -0.359
  HSO3-             0.000e+000  0.000e+000   -52.868   -52.959    -0.091
  H2SO3             0.000e+000  0.000e+000   -62.719   -62.719     0.000
  SO2               0.000e+000  0.000e+000   -62.965   -62.965     0.000
  S2O6-2            0.000e+000  0.000e+000   -79.131   -79.501    -0.370
  S3O6-2            0.000e+000  0.000e+000  -196.775  -197.145    -0.370
  S4O6-2            0.000e+000  0.000e+000  -298.172  -298.542    -0.370
  S5O6-2            0.000e+000  0.000e+000  -429.041  -429.412    -0.370
S(5)          0.000e+000
  S2O5-2            0.000e+000  0.000e+000  -110.357  -110.727    -0.370
S(6)          1.616e-002
  SO4-2             1.152e-002  4.913e-003    -1.938    -2.309    -0.370
  CaSO4             4.600e-003  4.600e-003    -2.337    -2.337     0.000
  NaSO4-            3.605e-005  2.925e-005    -4.443    -4.534    -0.091
  MgSO4             5.115e-006  5.115e-006    -5.291    -5.291     0.000
  KSO4-             2.673e-008  2.169e-008    -7.573    -7.664    -0.091
  HSO4-             7.537e-013  6.115e-013   -12.123   -12.214    -0.091
  LiSO4-            2.693e-015  2.185e-015   -14.570   -14.661    -0.091
  KHSO4             2.162e-020  2.162e-020   -19.665   -19.665     0.000
  H2SO4             1.213e-027  1.213e-027   -26.916   -26.916     0.000
  AlSO4+            1.899e-028  1.541e-028   -27.721   -27.812    -0.091
  Al(SO4)2-         7.242e-029  5.876e-029   -28.140   -28.231    -0.091
  FeSO4             4.316e-031  4.316e-031   -30.365   -30.365     0.000
  FeSO4+            3.458e-035  2.806e-035   -34.461   -34.552    -0.091
  Fe(SO4)2-         4.119e-036  3.342e-036   -35.385   -35.476    -0.091
S(7)          0.000e+000
  S2O8-2            0.000e+000  0.000e+000   -53.535   -53.905    -0.370
S(8)          6.281e-035
  HSO5-             6.281e-035  5.096e-035   -34.202   -34.293    -0.091
Si            4.777e-003
  HSiO3-            3.720e-003  3.018e-003    -2.429    -2.520    -0.091
  H2SiO4-2          5.864e-004  2.500e-004    -3.232    -3.602    -0.370
  NaHSiO3           1.542e-004  1.542e-004    -3.812    -3.812     0.000
  H4(H2SiO4)4-4     6.410e-005  2.085e-006    -4.193    -5.681    -1.488
  SiO2              5.917e-005  5.917e-005    -4.228    -4.228     0.000
  H6(H2SiO4)4-2     2.528e-007  1.078e-007    -6.597    -6.967    -0.370
```

## File 24. Mature Cement, Maximum ions, 95%/5% Mixing Ratio

*INPUT FILE*

```
SOLUTION 1
    temp      15
    pH        7.5 charge
    pe        4
    redox     pe
    units     mmol/kgw
    density   1
    Alkalinity 0
    Cl(-1)    7.5
    Li        1e-010
    Al        1e-010
    Ca        3.1
    Mg        5
    Na        18
    K         1.9
    S(6)      7.3
    N(5)      7.9
    C(4)      21.8
```

```
   Br(-1)    0
   Si        0.01
   -water    0.144 # kg

EQUILIBRIUM_PHASES 1
   Brucite   0 0.208
   Ca(OH)2*(CSH(1.5)) 0 1.42
   Calcite   0 0.001
   CSH(1.0-2.5) 0 2.386
   Ettringite 0 0.016
   Gibbsite  0 0.001
   Goethite  0 0.001
   Hydrogarnet(C3AH6) 0 0.384
   SiO2(am)  0 0.02
GAS_PHASE 1
   -fixed_pressure
   -pressure 1
   -volume 1
   -temperature 25
   CO2(g)    0.056
SAVE solution 1-1
END
SOLUTION 2
   temp      25
   pH        7.5 charge
   pe        4
   redox     pe
   units     mmol/kgw
   density   1
   Li        0
   Alkalinity 0
   Ca        3.1
   Mg        5
   Na        18
   C(4)      21.8
   Cl        7.5
   S(6)      7.3
   N(5)      7.9
   Si        0.001
   -water    0.144 # kg
GAS_PHASE 2
   -fixed_pressure
   -pressure 1
   -volume 1
   -temperature 25
   CO2(g)    0.056
   O2(g)     0.18
EQUILIBRIUM_PHASES 2
   calcite   0 1
SAVE solution 2-2
END
MIX 1
   1    0.95
   2    0.05
EQUILIBRIUM_PHASES 3
   Albite    0 0.6
   calcite   0 0.1
   K-Feldspar 0 0.6
   Quartz    0 72
   SiO2(am)  0 17.3
```

*SAMPLE OUTPUT, FINAL TIME STEP (FILE 24)*

```
-------------------------------------------
Beginning of batch-reaction calculations.
-------------------------------------------

Reaction step 1.

Using mix 1.
Using pure phase assemblage 3.

Mixture 1.

      9.500e-001 Solution 1       Solution after simulation 1.
      5.000e-002 Solution 2       Solution after simulation 2.

-------------------------------Phase assemblage--------------------------------

                                                    Moles in assemblage
Phase               SI log IAP  log KT      Initial       Final       Delta

Albite            0.00    2.93    2.93   6.000e-001  5.997e-001 -2.582e-004
Calcite           0.00    1.97    1.97   1.000e-001  1.002e-001  1.617e-004
K-Feldspar        0.00   -0.27   -0.27   6.000e-001  6.003e-001  2.583e-004
Quartz            0.00   -4.23   -4.23   7.200e+001  8.930e+001  1.730e+001
SiO2(am)         -1.36   -4.23   -2.87   1.730e+001           0 -1.730e+001

-----------------------------Solution composition------------------------------

      Elements          Molality       Moles

      Al              4.454e-007  6.430e-008
      C               7.746e-006  1.118e-006
      Ca              2.108e-002  3.043e-003
      Cl              7.481e-003  1.080e-003
      Fe              4.068e-009  5.872e-010
      K               1.156e-005  1.669e-006
      Li              9.477e-014  1.368e-014
      Mg              2.495e-004  3.601e-005
      N               7.881e-003  1.138e-003
      Na              1.974e-002  2.850e-003
      S               1.888e-002  2.726e-003
      Si              5.474e-003  7.902e-004

----------------------------Description of solution----------------------------

                                pH  =  11.691      Charge balance
                                pe  =   9.417      Adjusted to redox equilibrium
                     Activity of water  =   0.999
                        Ionic strength  =  7.930e-002
                    Mass of water (kg)  =  1.444e-001
                Total alkalinity (eq/kg)  =  9.290e-003
                    Total CO2 (mol/kg)  =  7.746e-006
                   Temperature (deg C)  =  15.500
                 Electrical balance (eq)  =  9.400e-013
Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   0.00
                           Iterations  =  18
                              Total H  = 1.603224e+001
                              Total O  = 8.032701e+000

---------------------------Distribution of species----------------------------
```

| Species | Molality | Log Activity | Log Molality | Log Activity | Gamma |
|---|---|---|---|---|---|
| OH- | 2.860e-003 | 2.250e-003 | -2.544 | -2.648 | -0.104 |
| H+ | 2.416e-012 | 2.035e-012 | -11.617 | -11.691 | -0.075 |
| H2O | 5.553e+001 | 9.987e-001 | 1.744 | -0.001 | 0.000 |
| Al | 4.454e-007 | | | | |
| AlO2- | 4.446e-007 | 3.526e-007 | -6.352 | -6.453 | -0.101 |
| NaAlO2 | 8.106e-010 | 8.106e-010 | -9.091 | -9.091 | 0.000 |
| HAlO2 | 3.403e-012 | 3.403e-012 | -11.468 | -11.468 | 0.000 |
| Al(OH)2+ | 1.109e-017 | 8.792e-018 | -16.955 | -17.056 | -0.101 |
| AlOH+2 | 3.684e-023 | 1.471e-023 | -22.434 | -22.832 | -0.399 |
| AlSO4+ | 3.472e-029 | 2.754e-029 | -28.459 | -28.560 | -0.101 |
| Al+3 | 2.558e-029 | 5.152e-030 | -28.592 | -29.288 | -0.696 |
| Al(SO4)2- | 1.408e-029 | 1.116e-029 | -28.851 | -28.952 | -0.101 |
| Al2(OH)2+4 | 0.000e+000 | 0.000e+000 | -41.379 | -42.884 | -1.506 |
| Al3(OH)4+5 | 0.000e+000 | 0.000e+000 | -52.696 | -54.981 | -2.285 |
| Al13O4(OH)24+7 | 0.000e+000 | 0.000e+000 | -100.882 | -105.362 | -4.481 |
| C(-2) | 0.000e+000 | | | | |
| C2H4 | 0.000e+000 | 0.000e+000 | -288.635 | -288.635 | 0.000 |
| C(-3) | 0.000e+000 | | | | |
| C2H6 | 0.000e+000 | 0.000e+000 | -259.769 | -259.769 | 0.000 |
| C(-4) | 0.000e+000 | | | | |
| CH4 | 0.000e+000 | 0.000e+000 | -159.628 | -159.628 | 0.000 |
| C(2) | 0.000e+000 | | | | |
| CO | 0.000e+000 | 0.000e+000 | -60.329 | -60.329 | 0.000 |
| C(4) | 7.746e-006 | | | | |
| CaCO3 | 6.353e-006 | 6.353e-006 | -5.197 | -5.197 | 0.000 |
| CO3-2 | 1.277e-006 | 5.100e-007 | -5.894 | -6.292 | -0.399 |
| NaCO3- | 3.941e-008 | 3.126e-008 | -7.404 | -7.505 | -0.101 |
| MgCO3 | 3.672e-008 | 3.672e-008 | -7.435 | -7.435 | 0.000 |
| HCO3- | 3.597e-008 | 2.853e-008 | -7.444 | -7.545 | -0.101 |
| CaHCO3+ | 2.827e-009 | 2.242e-009 | -8.549 | -8.649 | -0.101 |
| NaHCO3 | 6.702e-010 | 6.702e-010 | -9.174 | -9.174 | 0.000 |
| MgHCO3+ | 3.185e-011 | 2.526e-011 | -10.497 | -10.598 | -0.101 |
| CO2 | 1.521e-013 | 1.550e-013 | -12.818 | -12.810 | 0.008 |
| FeCO3+ | 1.949e-030 | 1.546e-030 | -29.710 | -29.811 | -0.101 |
| FeCO3 | 4.225e-032 | 4.225e-032 | -31.374 | -31.374 | 0.000 |
| FeHCO3+ | 2.258e-035 | 1.791e-035 | -34.646 | -34.747 | -0.101 |
| Ca | 2.108e-002 | | | | |
| Ca+2 | 1.551e-002 | 6.728e-003 | -1.809 | -2.172 | -0.363 |
| CaSO4 | 4.709e-003 | 4.709e-003 | -2.327 | -2.327 | 0.000 |
| CaOH+ | 5.882e-004 | 4.664e-004 | -3.231 | -3.331 | -0.101 |
| CaNO3+ | 2.528e-004 | 2.005e-004 | -3.597 | -3.698 | -0.101 |
| CaCl+ | 1.020e-005 | 8.086e-006 | -4.992 | -5.092 | -0.101 |
| CaCO3 | 6.353e-006 | 6.353e-006 | -5.197 | -5.197 | 0.000 |
| CaCl2 | 6.126e-008 | 6.126e-008 | -7.213 | -7.213 | 0.000 |
| CaHCO3+ | 2.827e-009 | 2.242e-009 | -8.549 | -8.649 | -0.101 |
| Cl(-1) | 7.481e-003 | | | | |
| Cl- | 7.458e-003 | 5.813e-003 | -2.127 | -2.236 | -0.108 |
| NaCl | 1.303e-005 | 1.303e-005 | -4.885 | -4.885 | 0.000 |
| CaCl+ | 1.020e-005 | 8.086e-006 | -4.992 | -5.092 | -0.101 |
| MgCl+ | 4.521e-007 | 3.586e-007 | -6.345 | -6.445 | -0.101 |
| CaCl2 | 6.126e-008 | 6.126e-008 | -7.213 | -7.213 | 0.000 |
| KCl | 1.388e-009 | 1.388e-009 | -8.858 | -8.858 | 0.000 |
| HCl | 2.611e-015 | 2.611e-015 | -14.583 | -14.583 | 0.000 |
| LiCl | 1.324e-017 | 1.324e-017 | -16.878 | -16.878 | 0.000 |
| FeCl+ | 6.150e-033 | 4.877e-033 | -32.211 | -32.312 | -0.101 |
| FeCl2+ | 1.264e-036 | 1.002e-036 | -35.898 | -35.999 | -0.101 |
| FeCl+2 | 3.276e-037 | 1.308e-037 | -36.485 | -36.883 | -0.399 |
| FeCl2 | 1.450e-037 | 1.450e-037 | -36.839 | -36.839 | 0.000 |
| FeCl4-2 | 0.000e+000 | 0.000e+000 | -40.443 | -40.855 | -0.412 |

```
  FeCl4-          0.000e+000  0.000e+000   -43.290   -43.390    -0.101
Cl(1)       1.603e-020
  ClO-          1.603e-020  1.271e-020   -19.795   -19.896    -0.101
  HClO           9.591e-025  9.591e-025   -24.018   -24.018     0.000
Cl(3)       5.732e-031
  ClO2-         5.732e-031  4.546e-031   -30.242   -30.342    -0.101
  HClO2          1.367e-039  1.367e-039   -38.864   -38.864     0.000
Cl(5)       4.181e-027
  ClO3-         4.181e-027  3.288e-027   -26.379   -26.483    -0.104
Cl(7)       1.280e-027
  ClO4-         1.280e-027  1.006e-027   -26.893   -26.997    -0.104
Fe(2)       1.882e-026
  Fe(OH)3-       1.784e-026  1.415e-026   -25.749   -25.849    -0.101
  Fe(OH)2        7.240e-028  7.240e-028   -27.140   -27.140     0.000
  FeOH+          2.341e-028  1.857e-028   -27.631   -27.731    -0.101
  Fe(OH)4-2      1.794e-029  6.944e-030   -28.746   -29.158    -0.412
  Fe+2           2.759e-030  1.196e-030   -29.559   -29.922    -0.363
  FeSO4          9.903e-031  9.903e-031   -30.004   -30.004     0.000
  FeCO3          4.225e-032  4.225e-032   -31.374   -31.374     0.000
  FeCl+          6.150e-033  4.877e-033   -32.211   -32.312    -0.101
  FeHCO3+        2.258e-035  1.791e-035   -34.646   -34.747    -0.101
  FeCl2          1.450e-037  1.450e-037   -36.839   -36.839     0.000
  FeCl4-2        0.000e+000  0.000e+000   -40.443   -40.855    -0.412
Fe(3)       4.068e-009
  Fe(OH)4-       4.042e-009  3.205e-009    -8.393    -8.494    -0.101
  Fe(OH)3        2.600e-011  2.600e-011   -10.585   -10.585     0.000
  Fe(OH)2+       1.428e-016  1.132e-016   -15.845   -15.946    -0.101
  FeOH+2         1.745e-024  6.967e-025   -23.758   -24.157    -0.399
  FeCO3+         1.949e-030  1.546e-030   -29.710   -29.811    -0.101
  Fe+3           1.092e-033  2.198e-034   -32.962   -33.658    -0.696
  FeSO4+         9.769e-035  7.748e-035   -34.010   -34.111    -0.101
  FeNO3+2        3.273e-035  1.307e-035   -34.485   -34.884    -0.399
  Fe(SO4)2-      1.237e-035  9.810e-036   -34.908   -35.008    -0.101
  FeCl2+         1.264e-036  1.002e-036   -35.898   -35.999    -0.101
  FeCl+2         3.276e-037  1.308e-037   -36.485   -36.883    -0.399
  FeCl4-         0.000e+000  0.000e+000   -43.290   -43.390    -0.101
  Fe2(OH)2+4     0.000e+000  0.000e+000   -45.378   -46.884    -1.506
  FeNO2+2        0.000e+000  0.000e+000   -45.952   -46.351    -0.399
  Fe3(OH)4+5     0.000e+000  0.000e+000   -58.225   -60.510    -2.285
H(0)        0.000e+000
  H2           0.000e+000  0.000e+000   -45.525   -45.516     0.008
K           1.156e-005
  K+           1.110e-005  8.654e-006    -4.955    -5.063    -0.108
  KSO4-          4.421e-007  3.506e-007    -6.354    -6.455    -0.101
  KOH            1.473e-008  1.473e-008    -7.832    -7.832     0.000
  KCl            1.388e-009  1.388e-009    -8.858    -8.858     0.000
  KHSO4          4.416e-019  4.416e-019   -18.355   -18.355     0.000
Li          9.477e-014
  Li+          9.104e-014  7.428e-014   -13.041   -13.129    -0.088
  LiSO4-         2.880e-015  2.284e-015   -14.541   -14.641    -0.101
  LiOH           8.352e-016  8.352e-016   -15.078   -15.078     0.000
  LiCl           1.324e-017  1.324e-017   -16.878   -16.878     0.000
Mg          2.495e-004
  Mg+2           1.643e-004  7.793e-005    -3.784    -4.108    -0.324
  MgSO4          8.461e-005  8.461e-005    -4.073    -4.073     0.000
  MgCl+          4.521e-007  3.586e-007    -6.345    -6.445    -0.101
  MgCO3          3.672e-008  3.672e-008    -7.435    -7.435     0.000
  Mg4(OH)4+4     1.220e-008  3.807e-010    -7.914    -9.419    -1.506
  MgHCO3+        3.185e-011  2.526e-011   -10.497   -10.598    -0.101
N(-03)      0.000e+000
  N3-          0.000e+000  0.000e+000  -105.101  -105.202    -0.101
  HN3            0.000e+000  0.000e+000  -112.103  -112.103     0.000
```

| | | | | | |
|---|---|---|---|---|---|
| N(-3) | 0.000e+000 | | | | |
| NH3 | 0.000e+000 | 0.000e+000 | -69.539 | -69.539 | 0.000 |
| NH4+ | 0.000e+000 | 0.000e+000 | -71.579 | -71.692 | -0.112 |
| NH4SO4- | 0.000e+000 | 0.000e+000 | -82.471 | -82.572 | -0.101 |
| N(0) | 1.381e-025 | | | | |
| N2 | 6.904e-026 | 6.904e-026 | -25.161 | -25.161 | 0.000 |
| N(3) | 1.843e-016 | | | | |
| NO2- | 1.843e-016 | 1.437e-016 | -15.734 | -15.843 | -0.108 |
| HNO2 | 6.112e-025 | 6.112e-025 | -24.214 | -24.214 | 0.000 |
| FeNO2+2 | 0.000e+000 | 0.000e+000 | -45.952 | -46.351 | -0.399 |
| N(5) | 7.881e-003 | | | | |
| NO3- | 7.628e-003 | 5.946e-003 | -2.118 | -2.226 | -0.108 |
| CaNO3+ | 2.528e-004 | 2.005e-004 | -3.597 | -3.698 | -0.101 |
| HNO3 | 5.038e-016 | 5.038e-016 | -15.298 | -15.298 | 0.000 |
| FeNO3+2 | 3.273e-035 | 1.307e-035 | -34.485 | -34.884 | -0.399 |
| Na | 1.974e-002 | | | | |
| Na+ | 1.728e-002 | 1.370e-002 | -1.763 | -1.863 | -0.101 |
| NaHSiO3 | 1.853e-003 | 1.853e-003 | -2.732 | -2.732 | 0.000 |
| NaSO4- | 5.962e-004 | 4.728e-004 | -3.225 | -3.325 | -0.101 |
| NaCl | 1.303e-005 | 1.303e-005 | -4.885 | -4.885 | 0.000 |
| NaOH | 5.442e-006 | 5.442e-006 | -5.264 | -5.264 | 0.000 |
| NaCO3- | 3.941e-008 | 3.126e-008 | -7.404 | -7.505 | -0.101 |
| NaAlO2 | 8.106e-010 | 8.106e-010 | -9.091 | -9.091 | 0.000 |
| NaHCO3 | 6.702e-010 | 6.702e-010 | -9.174 | -9.174 | 0.000 |
| O(0) | 9.075e-005 | | | | |
| O2 | 4.538e-005 | 4.626e-005 | -4.343 | -4.335 | 0.008 |
| S(-2) | 0.000e+000 | | | | |
| HS- | 0.000e+000 | 0.000e+000 | -148.478 | -148.582 | -0.104 |
| S-2 | 0.000e+000 | 0.000e+000 | -149.716 | -150.102 | -0.386 |
| H2S | 0.000e+000 | 0.000e+000 | -153.131 | -153.131 | 0.000 |
| S2-2 | 0.000e+000 | 0.000e+000 | -264.411 | -264.823 | -0.412 |
| S3-2 | 0.000e+000 | 0.000e+000 | -379.169 | -379.581 | -0.412 |
| S4-2 | 0.000e+000 | 0.000e+000 | -494.158 | -494.570 | -0.412 |
| S5-2 | 0.000e+000 | 0.000e+000 | -609.372 | -609.784 | -0.412 |
| S(2) | 0.000e+000 | | | | |
| S2O3-2 | 0.000e+000 | 0.000e+000 | -157.269 | -157.681 | -0.412 |
| HS2O3- | 0.000e+000 | 0.000e+000 | -168.258 | -168.358 | -0.101 |
| S(3) | 0.000e+000 | | | | |
| S2O4-2 | 0.000e+000 | 0.000e+000 | -143.739 | -144.125 | -0.386 |
| S(4) | 0.000e+000 | | | | |
| SO3-2 | 0.000e+000 | 0.000e+000 | -47.878 | -48.277 | -0.399 |
| HSO3- | 0.000e+000 | 0.000e+000 | -52.687 | -52.787 | -0.101 |
| H2SO3 | 0.000e+000 | 0.000e+000 | -62.446 | -62.446 | 0.000 |
| SO2 | 0.000e+000 | 0.000e+000 | -62.692 | -62.692 | 0.000 |
| S2O6-2 | 0.000e+000 | 0.000e+000 | -78.789 | -79.201 | -0.412 |
| S3O6-2 | 0.000e+000 | 0.000e+000 | -196.074 | -196.486 | -0.412 |
| S4O6-2 | 0.000e+000 | 0.000e+000 | -297.112 | -297.524 | -0.412 |
| S5O6-2 | 0.000e+000 | 0.000e+000 | -427.622 | -428.035 | -0.412 |
| S(5) | 0.000e+000 | | | | |
| S2O5-2 | 0.000e+000 | 0.000e+000 | -109.972 | -110.385 | -0.412 |
| S(6) | 1.888e-002 | | | | |
| SO4-2 | 1.349e-002 | 5.223e-003 | -1.870 | -2.282 | -0.412 |
| CaSO4 | 4.709e-003 | 4.709e-003 | -2.327 | -2.327 | 0.000 |
| NaSO4- | 5.962e-004 | 4.728e-004 | -3.225 | -3.325 | -0.101 |
| MgSO4 | 8.461e-005 | 8.461e-005 | -4.073 | -4.073 | 0.000 |
| KSO4- | 4.421e-007 | 3.506e-007 | -6.354 | -6.455 | -0.101 |
| HSO4- | 1.036e-012 | 8.218e-013 | -11.985 | -12.085 | -0.101 |
| LiSO4- | 2.880e-015 | 2.284e-015 | -14.541 | -14.641 | -0.101 |
| KHSO4 | 4.416e-019 | 4.416e-019 | -18.355 | -18.355 | 0.000 |
| H2SO4 | 2.061e-027 | 2.061e-027 | -26.686 | -26.686 | 0.000 |
| AlSO4+ | 3.472e-029 | 2.754e-029 | -28.459 | -28.560 | -0.101 |
| Al(SO4)2- | 1.408e-029 | 1.116e-029 | -28.851 | -28.952 | -0.101 |

```
   FeSO4              9.903e-031  9.903e-031   -30.004   -30.004     0.000
   FeSO4+             9.769e-035  7.748e-035   -34.010   -34.111    -0.101
   Fe(SO4)2-          1.237e-035  9.810e-036   -34.908   -35.008    -0.101
   NH4SO4-            0.000e+000  0.000e+000   -82.471   -82.572    -0.101
S(7)          0.000e+000
   S2O8-2             0.000e+000  0.000e+000   -53.279   -53.691    -0.412
S(8)          7.823e-035
   HSO5-              7.823e-035  6.204e-035   -34.107   -34.207    -0.101
Si            5.474e-003
   HSiO3-             3.009e-003  2.386e-003    -2.522    -2.622    -0.101
   NaHSiO3            1.853e-003  1.853e-003    -2.732    -2.732     0.000
   H2SiO4-2           4.038e-004  1.563e-004    -3.394    -3.806    -0.412
   SiO2               5.917e-005  5.917e-005    -4.228    -4.228     0.000
   H4(H2SiO4)4-4      3.700e-005  8.128e-007    -4.432    -6.090    -1.658
   H6(H2SiO4)4-2      1.735e-007  6.714e-008    -6.761    -7.173    -0.412
```

## File 25. Mature Cement, Minimum ions, 50%/50% Mixing Ratio

*INPUT FILE*

```
SOLUTION 1
   temp      15
   pH        7.5 charge
   pe        4
   redox     pe
   units     mmol/kgw
   density   1
   Alkalinity 0
   Cl(-1)    0.001
   Li        1e-010
   Al        1e-010
   Ca        0.6
   Mg        0.3
   Na        1.3
   K         0
   S(6)      0.3
   N(5)      0
   C(4)      1.4
   Br(-1)    0
   Si        0.01
   -water    0.144 # kg

EQUILIBRIUM_PHASES 1
   Brucite   0 0.208
   Ca(OH)2*(CSH(1.5)) 0 1.42
   Calcite   0 0.001
   CSH(1.0-2.5) 0 2.386
   Ettringite 0 0.016
   Gibbsite  0 0.001
   Goethite  0 0.001
   Hydrogarnet(C3AH6) 0 0.384
   SiO2(am)  0 0.02
GAS_PHASE 1
   -fixed_pressure
   -pressure 1
   -volume 1
   -temperature 25
   CO2(g)    0.056
SAVE solution 1-1
END
SOLUTION 2
   temp      25
```

```
    pH       7.5 charge
    pe       4
    redox    pe
    units    mmol/kgw
    density  1
    Li       0
    Alkalinity 0
    Ca       0.6
    Mg       0.3
    Na       1.3
    C(4)     1.4
    Cl       0.001
    S(6)     0.3
    N(5)     0
    Si       0.001
    K        0
    -water   0.144 # kg
GAS_PHASE 2
    -fixed_pressure
    -pressure 1
    -volume 1
    -temperature 25
    CO2(g)   0.056
    O2(g)    0.18
EQUILIBRIUM_PHASES 2
    calcite  0 1
SAVE solution 2-2
END
MIX 1
    1   0.5
    2   0.5
EQUILIBRIUM_PHASES 3
    Albite   0 0.6
    calcite  0 0.1
    K-Feldspar 0 0.6
    Quartz   0 72
    SiO2(am) 0 17.3
```

*SAMPLE OUTPUT, FINAL TIME STEP (FILE 25)*

```
-------------------------------------------
Beginning of batch-reaction calculations.
-------------------------------------------

Reaction step 1.

Using mix 1.
Using pure phase assemblage 3.

Mixture 1.

       5.000e-001 Solution 1       Solution after simulation 1.
       5.000e-001 Solution 2       Solution after simulation 2.

-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
Phase               SI log IAP  log KT     Initial      Final      Delta

Albite            -0.00    2.80    2.80   6.000e-001  5.999e-001 -7.298e-005
Calcite           -0.00    1.90    1.90   1.000e-001  1.006e-001  6.299e-004
K-Feldspar        -0.00   -0.32   -0.32   6.000e-001  6.000e-001 -1.989e-007
```

| | | | | | | |
|---|---|---|---|---|---|---|
| Quartz | 0.00 | -4.13 | -4.13 | 7.200e+001 | 8.930e+001 | 1.730e+001 |
| SiO2(am) | -1.32 | -4.13 | -2.81 | 1.730e+001 | 0 | -1.730e+001 |

----------Solution composition----------

| Elements | Molality | Moles |
|---|---|---|
| Al | 5.079e-004 | 7.325e-005 |
| C | 2.177e-003 | 3.139e-004 |
| Ca | 8.434e-003 | 1.216e-003 |
| Cl | 9.985e-007 | 1.440e-007 |
| Fe | 2.062e-009 | 2.973e-010 |
| K | 1.379e-006 | 1.989e-007 |
| Li | 4.993e-014 | 7.200e-015 |
| Mg | 1.498e-004 | 2.161e-005 |
| Na | 1.804e-003 | 2.602e-004 |
| S | 8.660e-003 | 1.249e-003 |
| Si | 7.428e-005 | 1.071e-005 |

----------Description of solution----------

| | |
|---|---|
| pH = | 7.156 Charge balance |
| pe = | 13.890 Adjusted to redox equilibrium |
| Activity of water = | 1.000 |
| Ionic strength = | 2.973e-002 |
| Mass of water (kg) = | 1.442e-001 |
| Total alkalinity (eq/kg) = | 3.176e-003 |
| Total CO2 (mol/kg) = | 2.177e-003 |
| Temperature (deg C) = | 20.000 |
| Electrical balance (eq) = | -3.224e-013 |
| Percent error, 100*(Cat-\|An\|)/(Cat+\|An\|) = | -0.00 |
| Iterations = | 16 |
| Total H = | 1.601539e+001 |
| Total O = | 8.013731e+000 |

----------Distribution of species----------

| Species | Molality | Log Activity | Log Molality | Log Activity | Gamma |
|---|---|---|---|---|---|
| OH- | 1.108e-007 | 9.393e-008 | -6.955 | -7.027 | -0.072 |
| H+ | 7.966e-008 | 6.989e-008 | -7.099 | -7.156 | -0.057 |
| H2O | 5.553e+001 | 9.997e-001 | 1.744 | -0.000 | 0.000 |
| Al | 5.079e-004 | | | | |
| Al13O4(OH)24+7 | 3.864e-005 | 2.423e-008 | -4.413 | -7.616 | -3.203 |
| AlO2- | 4.577e-006 | 3.893e-006 | -5.339 | -5.410 | -0.070 |
| HAlO2 | 1.019e-006 | 1.019e-006 | -5.992 | -5.992 | 0.000 |
| Al(OH)2+ | 7.913e-008 | 6.731e-008 | -7.102 | -7.172 | -0.070 |
| AlOH+2 | 5.371e-009 | 2.832e-009 | -8.270 | -8.548 | -0.278 |
| NaAlO2 | 1.039e-009 | 1.039e-009 | -8.983 | -8.983 | 0.000 |
| AlSO4+ | 1.055e-010 | 8.974e-011 | -9.977 | -10.047 | -0.070 |
| Al+3 | 8.251e-011 | 2.486e-011 | -10.084 | -10.605 | -0.521 |
| Al(SO4)2- | 2.889e-011 | 2.458e-011 | -10.539 | -10.609 | -0.070 |
| Al2(OH)2+4 | 3.013e-014 | 2.579e-015 | -13.521 | -14.589 | -1.067 |
| Al3(OH)4+5 | 3.639e-016 | 8.465e-018 | -15.439 | -17.072 | -1.633 |
| C(-2) | 0.000e+000 | | | | |
| C2H4 | 0.000e+000 | 0.000e+000 | -269.134 | -269.134 | 0.000 |
| C(-3) | 0.000e+000 | | | | |
| C2H6 | 0.000e+000 | 0.000e+000 | -241.198 | -241.198 | 0.000 |
| C(-4) | 0.000e+000 | | | | |
| CH4 | 0.000e+000 | 0.000e+000 | -150.133 | -150.133 | 0.000 |
| C(2) | 0.000e+000 | | | | |

| | | | | | | |
|---|---|---|---|---|---|---|
| CO | 0.000e+000 | 0.000e+000 | -50.838 | -50.838 | 0.000 | |
| C(4) | 2.177e-003 | | | | | |
| HCO3- | 1.820e-003 | 1.548e-003 | -2.740 | -2.810 | -0.070 | |
| CO2 | 2.669e-004 | 2.688e-004 | -3.574 | -3.571 | 0.003 | |
| CaHCO3+ | 7.703e-005 | 6.553e-005 | -4.113 | -4.184 | -0.070 | |
| CaCO3 | 6.614e-006 | 6.614e-006 | -5.180 | -5.180 | 0.000 | |
| NaHCO3 | 3.642e-006 | 3.642e-006 | -5.439 | -5.439 | 0.000 | |
| CO3-2 | 1.685e-006 | 8.885e-007 | -5.773 | -6.051 | -0.278 | |
| MgHCO3+ | 1.207e-006 | 1.027e-006 | -5.918 | -5.988 | -0.070 | |
| MgCO3 | 5.078e-008 | 5.078e-008 | -7.294 | -7.294 | 0.000 | |
| NaCO3- | 6.248e-009 | 5.316e-009 | -8.204 | -8.274 | -0.070 | |
| FeCO3+ | 5.619e-015 | 4.780e-015 | -14.250 | -14.321 | -0.070 | |
| FeHCO3+ | 8.992e-020 | 7.650e-020 | -19.046 | -19.116 | -0.070 | |
| FeCO3 | 5.253e-021 | 5.253e-021 | -20.280 | -20.280 | 0.000 | |
| Ca | 8.434e-003 | | | | | |
| Ca+2 | 6.572e-003 | 3.609e-003 | -2.182 | -2.443 | -0.260 | |
| CaSO4 | 1.779e-003 | 1.779e-003 | -2.750 | -2.750 | 0.000 | |
| CaHCO3+ | 7.703e-005 | 6.553e-005 | -4.113 | -4.184 | -0.070 | |
| CaCO3 | 6.614e-006 | 6.614e-006 | -5.180 | -5.180 | 0.000 | |
| CaOH+ | 8.570e-009 | 7.290e-009 | -8.067 | -8.137 | -0.070 | |
| CaCl+ | 7.457e-010 | 6.343e-010 | -9.127 | -9.198 | -0.070 | |
| CaCl2 | 6.616e-016 | 6.616e-016 | -15.179 | -15.179 | 0.000 | |
| Cl(-1) | 9.985e-007 | | | | | |
| Cl- | 9.975e-007 | 8.419e-007 | -6.001 | -6.075 | -0.074 | |
| CaCl+ | 7.457e-010 | 6.343e-010 | -9.127 | -9.198 | -0.070 | |
| NaCl | 2.133e-010 | 2.133e-010 | -9.671 | -9.671 | 0.000 | |
| MgCl+ | 4.496e-011 | 3.825e-011 | -10.347 | -10.417 | -0.070 | |
| KCl | 2.893e-014 | 2.893e-014 | -13.539 | -13.539 | 0.000 | |
| HCl | 1.313e-014 | 1.313e-014 | -13.882 | -13.882 | 0.000 | |
| CaCl2 | 6.616e-016 | 6.616e-016 | -15.179 | -15.179 | 0.000 | |
| LiCl | 1.124e-021 | 1.124e-021 | -20.949 | -20.949 | 0.000 | |
| FeCl+2 | 1.232e-025 | 6.495e-026 | -24.909 | -25.187 | -0.278 | |
| FeCl+ | 6.643e-026 | 5.651e-026 | -25.178 | -25.248 | -0.070 | |
| FeCl2+ | 6.711e-029 | 5.710e-029 | -28.173 | -28.243 | -0.070 | |
| FeCl2 | 2.487e-034 | 2.487e-034 | -33.604 | -33.604 | 0.000 | |
| FeCl4- | 0.000e+000 | 0.000e+000 | -43.243 | -43.313 | -0.070 | |
| FeCl4-2 | 0.000e+000 | 0.000e+000 | -45.015 | -45.299 | -0.284 | |
| Cl(1) | 3.696e-023 | | | | | |
| HClO | 2.542e-023 | 2.542e-023 | -22.595 | -22.595 | 0.000 | |
| ClO- | 1.153e-023 | 9.809e-024 | -22.938 | -23.008 | -0.070 | |
| Cl(3) | 1.946e-033 | | | | | |
| ClO2- | 1.946e-033 | 1.655e-033 | -32.711 | -32.781 | -0.070 | |
| HClO2 | 1.710e-037 | 1.710e-037 | -36.767 | -36.767 | 0.000 | |
| Cl(5) | 4.029e-029 | | | | | |
| ClO3- | 4.029e-029 | 3.414e-029 | -28.395 | -28.467 | -0.072 | |
| Cl(7) | 3.809e-029 | | | | | |
| ClO4- | 3.809e-029 | 3.228e-029 | -28.419 | -28.491 | -0.072 | |
| Fe(2) | 3.198e-019 | | | | | |
| Fe+2 | 1.715e-019 | 9.416e-020 | -18.766 | -19.026 | -0.260 | |
| FeHCO3+ | 8.992e-020 | 7.650e-020 | -19.046 | -19.116 | -0.070 | |
| FeSO4 | 5.265e-020 | 5.265e-020 | -19.279 | -19.279 | 0.000 | |
| FeCO3 | 5.253e-021 | 5.253e-021 | -20.280 | -20.280 | 0.000 | |
| FeOH+ | 5.006e-022 | 4.259e-022 | -21.300 | -21.371 | -0.070 | |
| FeCl+ | 6.643e-026 | 5.651e-026 | -25.178 | -25.248 | -0.070 | |
| Fe(OH)2 | 4.839e-026 | 4.839e-026 | -25.315 | -25.315 | 0.000 | |
| Fe(OH)3- | 3.239e-029 | 2.755e-029 | -28.490 | -28.560 | -0.070 | |
| FeCl2 | 2.487e-034 | 2.487e-034 | -33.604 | -33.604 | 0.000 | |
| Fe(OH)4-2 | 7.586e-037 | 3.941e-037 | -36.120 | -36.404 | -0.284 | |
| FeCl4-2 | 0.000e+000 | 0.000e+000 | -45.015 | -45.299 | -0.284 | |
| Fe(3) | 2.062e-009 | | | | | |
| Fe(OH)3 | 1.747e-009 | 1.747e-009 | -8.758 | -8.758 | 0.000 | |
| Fe(OH)2+ | 3.070e-010 | 2.612e-010 | -9.513 | -9.583 | -0.070 | |

| | | | | | |
|---|---|---|---|---|---|
| Fe(OH)4- | 7.379e-012 | 6.277e-012 | -11.132 | -11.202 | -0.070 |
| FeOH+2 | 1.046e-013 | 5.515e-014 | -12.980 | -13.258 | -0.278 |
| FeCO3+ | 5.619e-015 | 4.780e-015 | -14.250 | -14.321 | -0.070 |
| Fe+3 | 1.982e-018 | 5.972e-019 | -17.703 | -18.224 | -0.521 |
| FeSO4+ | 1.980e-019 | 1.684e-019 | -18.703 | -18.774 | -0.070 |
| Fe(SO4)2- | 1.429e-020 | 1.216e-020 | -19.845 | -19.915 | -0.070 |
| Fe2(OH)2+4 | 9.562e-025 | 8.185e-026 | -24.019 | -25.087 | -1.067 |
| FeCl+2 | 1.232e-025 | 6.495e-026 | -24.909 | -25.187 | -0.278 |
| FeCl2+ | 6.711e-029 | 5.710e-029 | -28.173 | -28.243 | -0.070 |
| Fe3(OH)4+5 | 1.920e-031 | 4.467e-033 | -30.717 | -32.350 | -1.633 |
| FeCl4- | 0.000e+000 | 0.000e+000 | -43.243 | -43.313 | -0.070 |
| H(0) | 0.000e+000 | | | | |
| H2 | 0.000e+000 | 0.000e+000 | -45.298 | -45.295 | 0.003 |
| K | 1.379e-006 | | | | |
| K+ | 1.342e-006 | 1.133e-006 | -5.872 | -5.946 | -0.074 |
| KSO4- | 3.710e-008 | 3.156e-008 | -7.431 | -7.501 | -0.070 |
| KOH | 5.618e-014 | 5.618e-014 | -13.250 | -13.250 | 0.000 |
| KCl | 2.893e-014 | 2.893e-014 | -13.539 | -13.539 | 0.000 |
| KHSO4 | 1.617e-015 | 1.617e-015 | -14.791 | -14.791 | 0.000 |
| Li | 4.993e-014 | | | | |
| Li+ | 4.890e-014 | 4.218e-014 | -13.311 | -13.375 | -0.064 |
| LiSO4- | 1.030e-015 | 8.763e-016 | -14.987 | -15.057 | -0.070 |
| LiOH | 1.382e-020 | 1.382e-020 | -19.859 | -19.859 | 0.000 |
| LiCl | 1.124e-021 | 1.124e-021 | -20.949 | -20.949 | 0.000 |
| Mg | 1.498e-004 | | | | |
| Mg+2 | 1.007e-004 | 5.796e-005 | -3.997 | -4.237 | -0.240 |
| MgSO4 | 4.787e-005 | 4.787e-005 | -4.320 | -4.320 | 0.000 |
| MgHCO3+ | 1.207e-006 | 1.027e-006 | -5.918 | -5.988 | -0.070 |
| MgCO3 | 5.078e-008 | 5.078e-008 | -7.294 | -7.294 | 0.000 |
| MgCl+ | 4.496e-011 | 3.825e-011 | -10.347 | -10.417 | -0.070 |
| Mg4(OH)4+4 | 9.807e-028 | 8.395e-029 | -27.008 | -28.076 | -1.067 |
| Na | 1.804e-003 | | | | |
| Na+ | 1.759e-003 | 1.497e-003 | -2.755 | -2.825 | -0.070 |
| NaSO4- | 4.101e-005 | 3.489e-005 | -4.387 | -4.457 | -0.070 |
| NaHCO3 | 3.642e-006 | 3.642e-006 | -5.439 | -5.439 | 0.000 |
| NaHSiO3 | 7.918e-009 | 7.918e-009 | -8.101 | -8.101 | 0.000 |
| NaCO3- | 6.248e-009 | 5.316e-009 | -8.204 | -8.274 | -0.070 |
| NaAlO2 | 1.039e-009 | 1.039e-009 | -8.983 | -8.983 | 0.000 |
| NaCl | 2.133e-010 | 2.133e-010 | -9.671 | -9.671 | 0.000 |
| NaOH | 2.452e-011 | 2.452e-011 | -10.610 | -10.610 | 0.000 |
| O(0) | 1.113e-003 | | | | |
| O2 | 5.563e-004 | 5.603e-004 | -3.255 | -3.252 | 0.003 |
| S(-2) | 0.000e+000 | | | | |
| HS- | 0.000e+000 | 0.000e+000 | -143.908 | -143.980 | -0.072 |
| H2S | 0.000e+000 | 0.000e+000 | -144.058 | -144.058 | 0.000 |
| S-2 | 0.000e+000 | 0.000e+000 | -149.626 | -149.898 | -0.272 |
| S2-2 | 0.000e+000 | 0.000e+000 | -255.394 | -255.679 | -0.284 |
| S3-2 | 0.000e+000 | 0.000e+000 | -361.215 | -361.499 | -0.284 |
| S4-2 | 0.000e+000 | 0.000e+000 | -467.264 | -467.549 | -0.284 |
| S5-2 | 0.000e+000 | 0.000e+000 | -573.535 | -573.820 | -0.284 |
| S(2) | 0.000e+000 | | | | |
| S2O3-2 | 0.000e+000 | 0.000e+000 | -148.461 | -148.745 | -0.284 |
| HS2O3- | 0.000e+000 | 0.000e+000 | -154.817 | -154.887 | -0.070 |
| S(3) | 0.000e+000 | | | | |
| S2O4-2 | 0.000e+000 | 0.000e+000 | -134.692 | -134.964 | -0.272 |
| S(4) | 0.000e+000 | | | | |
| SO3-2 | 0.000e+000 | 0.000e+000 | -47.967 | -48.245 | -0.278 |
| HSO3- | 0.000e+000 | 0.000e+000 | -48.126 | -48.197 | -0.070 |
| H2SO3 | 0.000e+000 | 0.000e+000 | -53.343 | -53.343 | 0.000 |
| SO2 | 0.000e+000 | 0.000e+000 | -53.521 | -53.521 | 0.000 |
| S2O6-2 | 0.000e+000 | 0.000e+000 | -69.741 | -70.025 | -0.284 |
| S3O6-2 | 0.000e+000 | 0.000e+000 | -178.066 | -178.351 | -0.284 |

```
  S4O6-2            0.000e+000  0.000e+000  -270.310  -270.594    -0.284
  S5O6-2            0.000e+000  0.000e+000  -391.740  -392.024    -0.284
S(5)          0.000e+000
  S2O5-2            0.000e+000  0.000e+000  -100.928  -101.212    -0.284
S(6)          8.660e-003
  SO4-2             6.792e-003  3.528e-003    -2.168    -2.452    -0.284
  CaSO4             1.779e-003  1.779e-003    -2.750    -2.750     0.000
  MgSO4             4.787e-005  4.787e-005    -4.320    -4.320     0.000
  NaSO4-            4.101e-005  3.489e-005    -4.387    -4.457    -0.070
  KSO4-             3.710e-008  3.156e-008    -7.431    -7.501    -0.070
  HSO4-             2.543e-008  2.163e-008    -7.595    -7.665    -0.070
  AlSO4+            1.055e-010  8.974e-011    -9.977   -10.047    -0.070
  Al(SO4)2-         2.889e-011  2.458e-011   -10.539   -10.609    -0.070
  KHSO4             1.617e-015  1.617e-015   -14.791   -14.791     0.000
  LiSO4-            1.030e-015  8.763e-016   -14.987   -15.057    -0.070
  H2SO4             1.643e-018  1.643e-018   -17.784   -17.784     0.000
  FeSO4+            1.980e-019  1.684e-019   -18.703   -18.774    -0.070
  FeSO4             5.265e-020  5.265e-020   -19.279   -19.279     0.000
  Fe(SO4)2-         1.429e-020  1.216e-020   -19.845   -19.915    -0.070
S(7)          0.000e+000
  S2O8-2            0.000e+000  0.000e+000   -43.595   -43.879    -0.284
S(8)          1.436e-029
  HSO5-             1.436e-029  1.222e-029   -28.843   -28.913    -0.070
Si            7.428e-005
  SiO2              7.415e-005  7.415e-005    -4.130    -4.130     0.000
  HSiO3-            1.199e-007  1.020e-007    -6.921    -6.991    -0.070
  NaHSiO3           7.918e-009  7.918e-009    -8.101    -8.101     0.000
  H2SiO4-2          3.202e-013  1.663e-013   -12.495   -12.779    -0.284
  H6(H2SiO4)4-2     2.722e-016  1.414e-016   -15.565   -15.850    -0.284
  H4(H2SiO4)4-4     2.009e-023  1.451e-024   -22.697   -23.838    -1.141
```

## File 26. Mature Cement, Maximum ions, 50%/50% Mixing Ratio

*INPUT FILE*

```
SOLUTION 1
    temp      15
    pH        7.5 charge
    pe        4
    redox     pe
    units     mmol/kgw
    density   1
    Alkalinity 0
    Cl(-1)    7.5
    Li        1e-010
    Al        1e-010
    Ca        3.1
    Mg        5
    Na        18
    K         1.9
    S(6)      7.3
    N(5)      7.9
    C(4)      21.8
    Br(-1)    0
    Si        0.01
    -water    0.144 # kg

EQUILIBRIUM_PHASES 1
    Brucite   0 0.208
    Ca(OH)2*(CSH(1.5)) 0 1.42
    Calcite   0 0.001
    CSH(1.0-2.5) 0 2.386
```

```
    Ettringite 0 0.016
    Gibbsite  0 0.001
    Goethite  0 0.001
    Hydrogarnet(C3AH6) 0 0.384
    SiO2(am)  0 0.02
GAS_PHASE 1
    -fixed_pressure
    -pressure 1
    -volume 1
    -temperature 25
    CO2(g)    0.056
SAVE solution 1-1
END
SOLUTION 2
    temp      25
    pH        7.5 charge
    pe        4
    redox     pe
    units     mmol/kgw
    density   1
    Li        0
    Alkalinity 0
    Ca        3.1
    Mg        5
    Na        18
    C(4)      21.8
    Cl        7.5
    S(6)      7.3
    N(5)      7.9
    Si        0.001
    K         1.9
    -water    0.144 # kg
GAS_PHASE 2
    -fixed_pressure
    -pressure 1
    -volume 1
    -temperature 25
    CO2(g)    0.056
    O2(g)     0.18
EQUILIBRIUM_PHASES 2
    calcite   0 1
SAVE solution 2-2
END
MIX 1
    1    0.5
    2    0.5
EQUILIBRIUM_PHASES 3
    Albite    0 0.6
    calcite   0 0.1
    K-Feldspar 0 0.6
    Quartz    0 72
    SiO2(am)  0 17.3
```

*SAMPLE OUTPUT, FINAL TIME STEP (FILE 26)*

```
-------------------------------------------
Beginning of batch-reaction calculations.
-------------------------------------------

Reaction step 1.

Using mix 1.
```

Using pure phase assemblage 3.

Mixture 1.

5.000e-001 Solution 1 Solution after simulation 1.
5.000e-001 Solution 2 Solution after simulation 2.

----------Phase assemblage----------

| Phase | SI | log IAP | log KT | Moles in assemblage: Initial | Final | Delta |
|---|---|---|---|---|---|---|
| Albite | 0.00 | 2.80 | 2.80 | 6.000e-001 | 5.997e-001 | -2.717e-004 |
| Calcite | 0.00 | 1.90 | 1.90 | 1.000e-001 | 1.005e-001 | 4.853e-004 |
| K-Feldspar | 0.00 | -0.32 | -0.32 | 6.000e-001 | 6.003e-001 | 2.714e-004 |
| Quartz | 0.00 | -4.13 | -4.13 | 7.200e+001 | 8.930e+001 | 1.730e+001 |
| SiO2(am) | -1.32 | -4.13 | -2.81 | 1.730e+001 | 0 | -1.730e+001 |

----------Solution composition----------

| Elements | Molality | Moles |
|---|---|---|
| Al | 2.444e-006 | 3.524e-007 |
| C | 7.921e-003 | 1.142e-003 |
| Ca | 1.150e-002 | 1.658e-003 |
| Cl | 7.490e-003 | 1.080e-003 |
| Fe | 2.143e-009 | 3.090e-010 |
| K | 1.523e-005 | 2.195e-006 |
| Li | 4.993e-014 | 7.200e-015 |
| Mg | 2.497e-003 | 3.600e-004 |
| N | 7.890e-003 | 1.138e-003 |
| Na | 1.986e-002 | 2.864e-003 |
| S | 1.340e-002 | 1.933e-003 |
| Si | 7.422e-005 | 1.070e-005 |

----------Description of solution----------

pH = 6.666 Charge balance
pe = 14.360 Adjusted to redox equilibrium
Activity of water = 0.999
Ionic strength = 6.068e-002
Mass of water (kg) = 1.442e-001
Total alkalinity (eq/kg) = 5.688e-003
Total CO2 (mol/kg) = 7.921e-003
Temperature (deg C) = 20.000
Electrical balance (eq) = 5.247e-013
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 0.00
Iterations = 16
Total H = 1.601327e+001
Total O = 8.020625e+000

----------Distribution of species----------

| Species | Molality | Log Activity | Log Molality | Log Activity | Gamma |
|---|---|---|---|---|---|
| H+ | 2.534e-007 | 2.157e-007 | -6.596 | -6.666 | -0.070 |
| OH- | 3.785e-008 | 3.041e-008 | -7.422 | -7.517 | -0.095 |
| H2O | 5.553e+001 | 9.989e-001 | 1.744 | -0.000 | 0.000 |
| Al | 2.444e-006 | | | | |
| AlO2- | 4.634e-007 | 3.749e-007 | -6.334 | -6.426 | -0.092 |
| HAlO2 | 3.029e-007 | 3.029e-007 | -6.519 | -6.519 | 0.000 |

| | | | | | |
|---|---|---|---|---|---|
| Al13O4(OH)24+7 | 1.215e-007 | 9.090e-012 | -6.915 | -11.041 | -4.126 |
| Al(OH)2+ | 7.632e-008 | 6.173e-008 | -7.117 | -7.209 | -0.092 |
| AlOH+2 | 1.857e-008 | 8.021e-009 | -7.731 | -8.096 | -0.365 |
| AlSO4+ | 1.131e-009 | 9.146e-010 | -8.947 | -9.039 | -0.092 |
| NaAlO2 | 1.039e-009 | 1.039e-009 | -8.983 | -8.983 | 0.000 |
| Al+3 | 9.701e-010 | 2.175e-010 | -9.013 | -9.663 | -0.649 |
| Al(SO4)2- | 3.607e-010 | 2.918e-010 | -9.443 | -9.535 | -0.092 |
| Al2(OH)2+4 | 5.003e-013 | 2.070e-014 | -12.301 | -13.684 | -1.383 |
| Al3(OH)4+5 | 7.914e-015 | 6.230e-017 | -14.102 | -16.206 | -2.104 |
| C(-2) | 0.000e+000 | | | | |
| C2H4 | 0.000e+000 | 0.000e+000 | -267.039 | -267.039 | 0.000 |
| C(-3) | 0.000e+000 | | | | |
| C2H6 | 0.000e+000 | 0.000e+000 | -239.064 | -239.064 | 0.000 |
| C(-4) | 0.000e+000 | | | | |
| CH4 | 0.000e+000 | 0.000e+000 | -149.046 | -149.046 | 0.000 |
| C(2) | 0.000e+000 | | | | |
| CO | 0.000e+000 | 0.000e+000 | -49.870 | -49.870 | 0.000 |
| C(4) | 7.921e-003 | | | | |
| HCO3- | 5.260e-003 | 4.255e-003 | -2.279 | -2.371 | -0.092 |
| CO2 | 2.249e-003 | 2.282e-003 | -2.648 | -2.642 | 0.006 |
| CaHCO3+ | 2.500e-004 | 2.022e-004 | -3.602 | -3.694 | -0.092 |
| NaHCO3 | 1.040e-004 | 1.040e-004 | -3.983 | -3.983 | 0.000 |
| MgHCO3+ | 4.961e-005 | 4.013e-005 | -4.304 | -4.397 | -0.092 |
| CaCO3 | 6.614e-006 | 6.614e-006 | -5.180 | -5.180 | 0.000 |
| CO3-2 | 1.832e-006 | 7.912e-007 | -5.737 | -6.102 | -0.365 |
| MgCO3 | 6.428e-007 | 6.428e-007 | -6.192 | -6.192 | 0.000 |
| NaCO3- | 6.078e-008 | 4.917e-008 | -7.216 | -7.308 | -0.092 |
| FeCO3+ | 1.209e-013 | 9.783e-014 | -12.917 | -13.010 | -0.092 |
| FeHCO3+ | 2.025e-018 | 1.638e-018 | -17.694 | -17.786 | -0.092 |
| FeCO3 | 3.644e-020 | 3.644e-020 | -19.438 | -19.438 | 0.000 |
| Ca | 1.150e-002 | | | | |
| Ca+2 | 8.755e-003 | 4.052e-003 | -2.058 | -2.392 | -0.335 |
| CaSO4 | 2.326e-003 | 2.326e-003 | -2.633 | -2.633 | 0.000 |
| CaHCO3+ | 2.500e-004 | 2.022e-004 | -3.602 | -3.694 | -0.092 |
| CaNO3+ | 1.549e-004 | 1.253e-004 | -3.810 | -3.902 | -0.092 |
| CaCO3 | 6.614e-006 | 6.614e-006 | -5.180 | -5.180 | 0.000 |
| CaCl+ | 6.226e-006 | 5.036e-006 | -5.206 | -5.298 | -0.092 |
| CaCl2 | 3.714e-008 | 3.714e-008 | -7.430 | -7.430 | 0.000 |
| CaOH+ | 3.277e-009 | 2.650e-009 | -8.485 | -8.577 | -0.092 |
| Cl(-1) | 7.490e-003 | | | | |
| Cl- | 7.463e-003 | 5.952e-003 | -2.127 | -2.225 | -0.098 |
| NaCl | 1.566e-005 | 1.566e-005 | -4.805 | -4.805 | 0.000 |
| CaCl+ | 6.226e-006 | 5.036e-006 | -5.206 | -5.298 | -0.092 |
| MgCl+ | 4.752e-006 | 3.844e-006 | -5.323 | -5.415 | -0.092 |
| CaCl2 | 3.714e-008 | 3.714e-008 | -7.430 | -7.430 | 0.000 |
| KCl | 2.125e-009 | 2.125e-009 | -8.673 | -8.673 | 0.000 |
| HCl | 2.864e-010 | 2.864e-010 | -9.543 | -9.543 | 0.000 |
| LiCl | 7.604e-018 | 7.604e-018 | -17.119 | -17.119 | 0.000 |
| FeCl2+ | 8.108e-020 | 6.559e-020 | -19.091 | -19.183 | -0.092 |
| FeCl+2 | 2.443e-020 | 1.055e-020 | -19.612 | -19.977 | -0.365 |
| FeCl+ | 3.848e-021 | 3.113e-021 | -20.415 | -20.507 | -0.092 |
| FeCl2 | 9.686e-026 | 9.686e-026 | -25.014 | -25.014 | 0.000 |
| FeCl4- | 3.454e-027 | 2.794e-027 | -26.462 | -26.554 | -0.092 |
| FeCl4-2 | 2.322e-029 | 9.776e-030 | -28.634 | -29.010 | -0.376 |
| Cl(1) | 5.846e-019 | | | | |
| HClO | 5.064e-019 | 5.064e-019 | -18.296 | -18.296 | 0.000 |
| ClO- | 7.825e-020 | 6.330e-020 | -19.106 | -19.199 | -0.092 |
| Cl(3) | 1.206e-029 | | | | |
| ClO2- | 1.205e-029 | 9.749e-030 | -28.919 | -29.011 | -0.092 |
| HClO2 | 3.109e-033 | 3.109e-033 | -32.507 | -32.507 | 0.000 |
| Cl(5) | 2.285e-025 | | | | |
| ClO3- | 2.285e-025 | 1.835e-025 | -24.641 | -24.736 | -0.095 |

| | | | | | |
|---|---|---|---|---|---|
| Cl(7) | 1.972e-025 | | | | |
| ClO4- | 1.972e-025 | 1.584e-025 | -24.705 | -24.800 | -0.095 |
| Fe(2) | 4.129e-018 | | | | |
| FeHCO3+ | 2.025e-018 | 1.638e-018 | -17.694 | -17.786 | -0.092 |
| Fe+2 | 1.585e-018 | 7.336e-019 | -17.800 | -18.135 | -0.335 |
| FeSO4 | 4.778e-019 | 4.778e-019 | -18.321 | -18.321 | 0.000 |
| FeCO3 | 3.644e-020 | 3.644e-020 | -19.438 | -19.438 | 0.000 |
| FeCl+ | 3.848e-021 | 3.113e-021 | -20.415 | -20.507 | -0.092 |
| FeOH+ | 1.328e-021 | 1.074e-021 | -20.877 | -20.969 | -0.092 |
| FeCl2 | 9.686e-026 | 9.686e-026 | -25.014 | -25.014 | 0.000 |
| Fe(OH)2 | 3.951e-026 | 3.951e-026 | -25.403 | -25.403 | 0.000 |
| FeCl4-2 | 2.322e-029 | 9.776e-030 | -28.634 | -29.010 | -0.376 |
| Fe(OH)3- | 9.004e-030 | 7.283e-030 | -29.046 | -29.138 | -0.092 |
| Fe(OH)4-2 | 8.011e-038 | 3.373e-038 | -37.096 | -37.472 | -0.376 |
| Fe(3) | 2.143e-009 | | | | |
| Fe(OH)3 | 1.363e-009 | 1.363e-009 | -8.866 | -8.866 | 0.000 |
| Fe(OH)2+ | 7.777e-010 | 6.291e-010 | -9.109 | -9.201 | -0.092 |
| Fe(OH)4- | 1.959e-012 | 1.585e-012 | -11.708 | -11.800 | -0.092 |
| FeOH+2 | 9.498e-013 | 4.103e-013 | -12.022 | -12.387 | -0.365 |
| FeCO3+ | 1.209e-013 | 9.783e-014 | -12.917 | -13.010 | -0.092 |
| Fe+3 | 6.121e-017 | 1.372e-017 | -16.213 | -16.863 | -0.649 |
| FeSO4+ | 5.573e-018 | 4.508e-018 | -17.254 | -17.346 | -0.092 |
| FeNO3+2 | 1.960e-018 | 8.465e-019 | -17.708 | -18.072 | -0.365 |
| Fe(SO4)2- | 4.687e-019 | 3.791e-019 | -18.329 | -18.421 | -0.092 |
| FeCl2+ | 8.108e-020 | 6.559e-020 | -19.091 | -19.183 | -0.092 |
| FeCl+2 | 2.443e-020 | 1.055e-020 | -19.612 | -19.977 | -0.365 |
| Fe2(OH)2+4 | 1.095e-022 | 4.531e-024 | -21.961 | -23.344 | -1.383 |
| FeCl4- | 3.454e-027 | 2.794e-027 | -26.462 | -26.554 | -0.092 |
| Fe3(OH)4+5 | 7.565e-029 | 5.955e-031 | -28.121 | -30.225 | -2.104 |
| FeNO2+2 | 3.876e-030 | 1.674e-030 | -29.412 | -29.776 | -0.365 |
| H(0) | 0.000e+000 | | | | |
| H2 | 0.000e+000 | 0.000e+000 | -45.262 | -45.256 | 0.006 |
| K | 1.523e-005 | | | | |
| K+ | 1.475e-005 | 1.177e-005 | -4.831 | -4.929 | -0.098 |
| KSO4- | 4.720e-007 | 3.818e-007 | -6.326 | -6.418 | -0.092 |
| KCl | 2.125e-009 | 2.125e-009 | -8.673 | -8.673 | 0.000 |
| KOH | 1.889e-013 | 1.889e-013 | -12.724 | -12.724 | 0.000 |
| KHSO4 | 6.036e-014 | 6.036e-014 | -13.219 | -13.219 | 0.000 |
| Li | 4.993e-014 | | | | |
| Li+ | 4.872e-014 | 4.035e-014 | -13.312 | -13.394 | -0.082 |
| LiSO4- | 1.207e-015 | 9.765e-016 | -14.918 | -15.010 | -0.092 |
| LiCl | 7.604e-018 | 7.604e-018 | -17.119 | -17.119 | 0.000 |
| LiOH | 4.281e-021 | 4.281e-021 | -20.368 | -20.368 | 0.000 |
| Mg | 2.497e-003 | | | | |
| Mg+2 | 1.649e-003 | 8.238e-004 | -2.783 | -3.084 | -0.301 |
| MgSO4 | 7.925e-004 | 7.925e-004 | -3.101 | -3.101 | 0.000 |
| MgHCO3+ | 4.961e-005 | 4.013e-005 | -4.304 | -4.397 | -0.092 |
| MgCl+ | 4.752e-006 | 3.844e-006 | -5.323 | -5.415 | -0.092 |
| MgCO3 | 6.428e-007 | 6.428e-007 | -6.192 | -6.192 | 0.000 |
| Mg4(OH)4+4 | 9.100e-025 | 3.765e-026 | -24.041 | -25.424 | -1.383 |
| N(-03) | 0.000e+000 | | | | |
| N3- | 0.000e+000 | 0.000e+000 | -97.478 | -97.571 | -0.092 |
| HN3 | 0.000e+000 | 0.000e+000 | -99.489 | -99.489 | 0.000 |
| N(-3) | 0.000e+000 | | | | |
| NH4+ | 0.000e+000 | 0.000e+000 | -62.607 | -62.708 | -0.102 |
| NH3 | 0.000e+000 | 0.000e+000 | -65.437 | -65.437 | 0.000 |
| NH4SO4- | 0.000e+000 | 0.000e+000 | -73.457 | -73.549 | -0.092 |
| N(0) | 8.756e-018 | | | | |
| N2 | 4.378e-018 | 4.378e-018 | -17.359 | -17.359 | 0.000 |
| N(3) | 1.083e-016 | | | | |
| NO2- | 1.083e-016 | 8.638e-017 | -15.965 | -16.064 | -0.098 |
| HNO2 | 3.530e-020 | 3.530e-020 | -19.452 | -19.452 | 0.000 |

| | | | | | |
|---|---|---|---|---|---|
| FeNO2+2 | 3.876e-030 | 1.674e-030 | -29.412 | -29.776 | -0.365 |
| N(5) | 7.890e-003 | | | | |
| NO3- | 7.735e-003 | 6.169e-003 | -2.112 | -2.210 | -0.098 |
| CaNO3+ | 1.549e-004 | 1.253e-004 | -3.810 | -3.902 | -0.092 |
| HNO3 | 6.179e-011 | 6.179e-011 | -10.209 | -10.209 | 0.000 |
| FeNO3+2 | 1.960e-018 | 8.465e-019 | -17.708 | -18.072 | -0.365 |
| Na | 1.986e-002 | | | | |
| Na+ | 1.922e-002 | 1.555e-002 | -1.716 | -1.808 | -0.092 |
| NaSO4- | 5.218e-004 | 4.221e-004 | -3.282 | -3.375 | -0.092 |
| NaHCO3 | 1.040e-004 | 1.040e-004 | -3.983 | -3.983 | 0.000 |
| NaCl | 1.566e-005 | 1.566e-005 | -4.805 | -4.805 | 0.000 |
| NaCO3- | 6.078e-008 | 4.917e-008 | -7.216 | -7.308 | -0.092 |
| NaHSiO3 | 2.662e-008 | 2.662e-008 | -7.575 | -7.575 | 0.000 |
| NaAlO2 | 1.039e-009 | 1.039e-009 | -8.983 | -8.983 | 0.000 |
| NaOH | 8.246e-011 | 8.246e-011 | -10.084 | -10.084 | 0.000 |
| O(0) | 9.199e-004 | | | | |
| O2 | 4.600e-004 | 4.668e-004 | -3.337 | -3.331 | 0.006 |
| S(-2) | 0.000e+000 | | | | |
| H2S | 0.000e+000 | 0.000e+000 | -142.854 | -142.854 | 0.000 |
| HS- | 0.000e+000 | 0.000e+000 | -143.170 | -143.266 | -0.095 |
| S-2 | 0.000e+000 | 0.000e+000 | -149.319 | -149.673 | -0.354 |
| S2-2 | 0.000e+000 | 0.000e+000 | -253.914 | -254.289 | -0.376 |
| S3-2 | 0.000e+000 | 0.000e+000 | -358.569 | -358.945 | -0.376 |
| S4-2 | 0.000e+000 | 0.000e+000 | -463.455 | -463.831 | -0.376 |
| S5-2 | 0.000e+000 | 0.000e+000 | -568.561 | -568.937 | -0.376 |
| S(2) | 0.000e+000 | | | | |
| S2O3-2 | 0.000e+000 | 0.000e+000 | -147.099 | -147.475 | -0.376 |
| HS2O3- | 0.000e+000 | 0.000e+000 | -153.035 | -153.127 | -0.092 |
| S(3) | 0.000e+000 | | | | |
| S2O4-2 | 0.000e+000 | 0.000e+000 | -133.379 | -133.733 | -0.354 |
| S(4) | 0.000e+000 | | | | |
| HSO3- | 0.000e+000 | 0.000e+000 | -47.509 | -47.601 | -0.092 |
| SO3-2 | 0.000e+000 | 0.000e+000 | -47.775 | -48.139 | -0.365 |
| H2SO3 | 0.000e+000 | 0.000e+000 | -52.258 | -52.258 | 0.000 |
| SO2 | 0.000e+000 | 0.000e+000 | -52.436 | -52.436 | 0.000 |
| S2O6-2 | 0.000e+000 | 0.000e+000 | -68.498 | -68.874 | -0.376 |
| S3O6-2 | 0.000e+000 | 0.000e+000 | -175.659 | -176.035 | -0.376 |
| S4O6-2 | 0.000e+000 | 0.000e+000 | -266.738 | -267.114 | -0.376 |
| S5O6-2 | 0.000e+000 | 0.000e+000 | -387.004 | -387.379 | -0.376 |
| S(5) | 0.000e+000 | | | | |
| S2O5-2 | 0.000e+000 | 0.000e+000 | -99.646 | -100.021 | -0.376 |
| S(6) | 1.340e-002 | | | | |
| SO4-2 | 9.762e-003 | 4.110e-003 | -2.010 | -2.386 | -0.376 |
| CaSO4 | 2.326e-003 | 2.326e-003 | -2.633 | -2.633 | 0.000 |
| MgSO4 | 7.925e-004 | 7.925e-004 | -3.101 | -3.101 | 0.000 |
| NaSO4- | 5.218e-004 | 4.221e-004 | -3.282 | -3.375 | -0.092 |
| KSO4- | 4.720e-007 | 3.818e-007 | -6.326 | -6.418 | -0.092 |
| HSO4- | 9.614e-008 | 7.777e-008 | -7.017 | -7.109 | -0.092 |
| AlSO4+ | 1.131e-009 | 9.146e-010 | -8.947 | -9.039 | -0.092 |
| Al(SO4)2- | 3.607e-010 | 2.918e-010 | -9.443 | -9.535 | -0.092 |
| KHSO4 | 6.036e-014 | 6.036e-014 | -13.219 | -13.219 | 0.000 |
| LiSO4- | 1.207e-015 | 9.765e-016 | -14.918 | -15.010 | -0.092 |
| H2SO4 | 1.822e-017 | 1.822e-017 | -16.739 | -16.739 | 0.000 |
| FeSO4+ | 5.573e-018 | 4.508e-018 | -17.254 | -17.346 | -0.092 |
| FeSO4 | 4.778e-019 | 4.778e-019 | -18.321 | -18.321 | 0.000 |
| Fe(SO4)2- | 4.687e-019 | 3.791e-019 | -18.329 | -18.421 | -0.092 |
| NH4SO4- | 0.000e+000 | 0.000e+000 | -73.457 | -73.549 | -0.092 |
| S(7) | 0.000e+000 | | | | |
| S2O8-2 | 0.000e+000 | 0.000e+000 | -42.431 | -42.807 | -0.376 |
| S(8) | 4.956e-029 | | | | |
| HSO5- | 4.956e-029 | 4.009e-029 | -28.305 | -28.397 | -0.092 |
| Si | 7.422e-005 | | | | |

```
SiO2              7.415e-005  7.415e-005   -4.130   -4.130    0.000
HSiO3-            4.082e-008  3.302e-008   -7.389   -7.481   -0.092
NaHSiO3           2.662e-008  2.662e-008   -7.575   -7.575    0.000
H2SiO4-2          4.141e-014  1.743e-014  -13.383  -13.759   -0.376
H6(H2SiO4)4-2     3.503e-017  1.475e-017  -16.456  -16.831   -0.376
H4(H2SiO4)4-4     5.144e-025  1.589e-026  -24.289  -25.799   -1.510
```

## File 27. Degraded Cement, Minimum ions, 95%/5% Mixing Ratio

*INPUT FILE*

```
SOLUTION 1
   temp      15
   pH       7.5 charge
   pe       4
   redox     pe
   units     mmol/kgw
   density   1
   Alkalinity 0
   Cl(-1)    0
   Li        1e-010
   Al        1e-010
   Ca        0.6
   Mg        0.3
   Na        1.3
   K         0
   S(6)      0.3
   N(5)      0
   C(4)      1.4
   Br(-1)    0
   Si        0.01
   -water    0.144 # kg

EQUILIBRIUM_PHASES 1
   Brucite   0 1.39
   Calcite   0 9.5
   Gibbsite  0 1e-010
   Goethite  0 0.001
   SiO2(am)  0 4
   CSH(0.25) 0 12
GAS_PHASE 1
   -fixed_pressure
   -pressure 1
   -volume 1
   -temperature 25
   CO2(g)    0.056
SAVE solution 1-1
END
SOLUTION 2
   temp      25
   pH       7.5 charge
   pe       4
   redox     pe
   units     mmol/kgs
   density   1
   Li        0
   Alkalinity 0
   Ca        3.1
   Mg        5
   Na        18
   C(4)      21.8
   Cl        7.5
```

```
   S(6)      7.3
   N(5)      7.8
   Si        0.001
   K         1.9
   -water    0.144 # kg
GAS_PHASE 2
   -fixed_pressure
   -pressure 1
   -volume 1
   -temperature 25
   CO2(g)    0.056
   O2(g)     0.18
EQUILIBRIUM_PHASES 2
   calcite   0 1
SAVE solution 2-2
END
MIX 1
   1    0.95
   2    0.05
EQUILIBRIUM_PHASES 3
   Albite    0 0.6
   Calcite   0 0.1
   K-Feldspar 0 0.6
   Quartz    0 72
   SiO2(am)  0 17.3
```

*SAMPLE OUTPUT, FINAL TIME STEP (FILE 27)*

```
-------------------------------------------
Beginning of batch-reaction calculations.
-------------------------------------------

Reaction step 1.

WARNING: Maximum iterations exceeded, 100

WARNING: Numerical method failed with this set of convergence parameters.

WARNING: Trying smaller step size, pe step size 10, 5 ...

Using mix 1.
Using pure phase assemblage 3.

Mixture 1.

       9.500e-001 Solution 1       Solution after simulation 1.
       5.000e-002 Solution 2       Solution after simulation 2.

-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
Phase               SI log IAP  log KT      Initial       Final       Delta

Albite            -0.00    2.93    2.93   6.000e-001  6.000e-001 -1.391e-005
Calcite            0.00    1.97    1.97   1.000e-001  1.002e-001  1.614e-004
K-Feldspar        -0.00   -0.27   -0.27   6.000e-001  6.000e-001  1.353e-005
Quartz             0.00   -4.23   -4.23   7.200e+001  8.930e+001  1.730e+001
SiO2(am)          -1.36   -4.23   -2.87   1.730e+001           0 -1.730e+001

-----------------------------Solution composition------------------------------

       Elements           Molality       Moles
```

| | | |
|---|---|---|
| Al | 2.638e-006 | 3.800e-007 |
| C | 2.567e-005 | 3.698e-006 |
| Ca | 4.662e-004 | 6.715e-005 |
| Cl | 3.761e-004 | 5.417e-005 |
| Fe | 6.377e-011 | 9.186e-012 |
| K | 1.356e-006 | 1.953e-007 |
| Li | 9.497e-014 | 1.368e-014 |
| Mg | 4.183e-004 | 6.025e-005 |
| N | 3.911e-004 | 5.634e-005 |
| Na | 2.234e-003 | 3.218e-004 |
| S | 6.510e-004 | 9.377e-005 |
| Si | 1.068e-003 | 1.538e-004 |

----------Description of solution----------

pH = 11.230 Charge balance
pe = 9.879 Adjusted to redox equilibrium
Activity of water = 1.000
Ionic strength = 5.245e-003
Mass of water (kg) = 1.440e-001
Total alkalinity (eq/kg) = 1.943e-003
Total CO2 (mol/kg) = 2.567e-005
Temperature (deg C) = 15.500
Electrical balance (eq) = 5.890e-014
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 0.00
Iterations = 30
Total H = 1.599631e+001
Total O = 7.999169e+000

----------Distribution of species----------

| Species | Molality | Log Activity | Log Molality | Log Activity | Gamma |
|---|---|---|---|---|---|
| OH- | 8.403e-004 | 7.778e-004 | -3.076 | -3.109 | -0.034 |
| H+ | 6.312e-012 | 5.892e-012 | -11.200 | -11.230 | -0.030 |
| H2O | 5.553e+001 | 9.999e-001 | 1.744 | -0.000 | 0.000 |
| Al | 2.638e-006 | | | | |
| AlO2- | 2.637e-006 | 2.443e-006 | -5.579 | -5.612 | -0.033 |
| NaAlO2 | 8.106e-010 | 8.106e-010 | -9.091 | -9.091 | 0.000 |
| HAlO2 | 6.826e-011 | 6.826e-011 | -10.166 | -10.166 | 0.000 |
| Al(OH)2+ | 5.513e-016 | 5.108e-016 | -15.259 | -15.292 | -0.033 |
| AlOH+2 | 3.349e-021 | 2.472e-021 | -20.475 | -20.607 | -0.132 |
| Al+3 | 4.672e-027 | 2.504e-027 | -26.330 | -26.601 | -0.271 |
| AlSO4+ | 1.218e-027 | 1.129e-027 | -26.914 | -26.947 | -0.033 |
| Al(SO4)2- | 4.167e-029 | 3.860e-029 | -28.380 | -28.413 | -0.033 |
| Al2(OH)2+4 | 1.212e-038 | 3.684e-039 | -37.916 | -38.434 | -0.517 |
| Al3(OH)4+5 | 0.000e+000 | 0.000e+000 | -47.966 | -48.766 | -0.800 |
| Al13O4(OH)24+7 | 0.000e+000 | 0.000e+000 | -83.630 | -85.198 | -1.568 |
| C(-2) | 0.000e+000 | | | | |
| C2H4 | 0.000e+000 | 0.000e+000 | -284.143 | -284.143 | 0.000 |
| C(-3) | 0.000e+000 | | | | |
| C2H6 | 0.000e+000 | 0.000e+000 | -255.276 | -255.276 | 0.000 |
| C(-4) | 0.000e+000 | | | | |
| CH4 | 0.000e+000 | 0.000e+000 | -157.381 | -157.381 | 0.000 |
| C(2) | 0.000e+000 | | | | |
| CO | 0.000e+000 | 0.000e+000 | -58.085 | -58.085 | 0.000 |
| C(4) | 2.567e-005 | | | | |
| CO3-2 | 1.445e-005 | 1.066e-005 | -4.840 | -4.972 | -0.132 |
| CaCO3 | 6.353e-006 | 6.353e-006 | -5.197 | -5.197 | 0.000 |
| MgCO3 | 2.885e-006 | 2.885e-006 | -5.540 | -5.540 | 0.000 |

| | | | | | |
|---|---|---|---|---|---|
| HCO3- | 1.864e-006 | 1.727e-006 | -5.729 | -5.763 | -0.033 |
| NaCO3- | 1.018e-007 | 9.432e-008 | -6.992 | -7.025 | -0.033 |
| CaHCO3+ | 7.009e-009 | 6.493e-009 | -8.154 | -8.188 | -0.033 |
| MgHCO3+ | 6.204e-009 | 5.747e-009 | -8.207 | -8.241 | -0.033 |
| NaHCO3 | 5.857e-009 | 5.857e-009 | -8.232 | -8.232 | 0.000 |
| CO2 | 2.711e-011 | 2.715e-011 | -10.567 | -10.566 | 0.001 |
| FeCO3+ | 4.404e-029 | 4.080e-029 | -28.356 | -28.389 | -0.033 |
| FeCO3 | 3.857e-031 | 3.857e-031 | -30.414 | -30.414 | 0.000 |
| FeHCO3+ | 5.110e-034 | 4.734e-034 | -33.292 | -33.325 | -0.033 |
| Ca | 4.662e-004 | | | | |
| Ca+2 | 4.319e-004 | 3.218e-004 | -3.365 | -3.492 | -0.128 |
| CaSO4 | 1.900e-005 | 1.900e-005 | -4.721 | -4.721 | 0.000 |
| CaOH+ | 8.326e-006 | 7.714e-006 | -5.080 | -5.113 | -0.033 |
| CaCO3 | 6.353e-006 | 6.353e-006 | -5.197 | -5.197 | 0.000 |
| CaNO3+ | 6.287e-007 | 5.824e-007 | -6.202 | -6.235 | -0.033 |
| CaCl+ | 2.496e-008 | 2.313e-008 | -7.603 | -7.636 | -0.033 |
| CaHCO3+ | 7.009e-009 | 6.493e-009 | -8.154 | -8.188 | -0.033 |
| CaCl2 | 1.048e-011 | 1.048e-011 | -10.980 | -10.980 | 0.000 |
| Cl(-1) | 3.761e-004 | | | | |
| Cl- | 3.758e-004 | 3.476e-004 | -3.425 | -3.459 | -0.034 |
| NaCl | 1.124e-007 | 1.124e-007 | -6.949 | -6.949 | 0.000 |
| MgCl+ | 8.698e-008 | 8.058e-008 | -7.061 | -7.094 | -0.033 |
| CaCl+ | 2.496e-008 | 2.313e-008 | -7.603 | -7.636 | -0.033 |
| KCl | 1.198e-011 | 1.198e-011 | -10.922 | -10.922 | 0.000 |
| CaCl2 | 1.048e-011 | 1.048e-011 | -10.980 | -10.980 | 0.000 |
| HCl | 4.520e-016 | 4.520e-016 | -15.345 | -15.345 | 0.000 |
| LiCl | 9.349e-019 | 9.349e-019 | -18.029 | -18.029 | 0.000 |
| FeCl+ | 1.374e-034 | 1.273e-034 | -33.862 | -33.895 | -0.033 |
| FeCl+2 | 1.338e-038 | 9.874e-039 | -37.874 | -38.005 | -0.132 |
| FeCl2+ | 4.883e-039 | 4.524e-039 | -38.311 | -38.344 | -0.033 |
| FeCl2 | 2.263e-040 | 2.263e-040 | -39.645 | -39.645 | 0.000 |
| FeCl4-2 | 0.000e+000 | 0.000e+000 | -45.975 | -46.108 | -0.133 |
| FeCl4- | 0.000e+000 | 0.000e+000 | -48.149 | -48.182 | -0.033 |
| Cl(1) | 8.192e-022 | | | | |
| ClO- | 8.190e-022 | 7.588e-022 | -21.087 | -21.120 | -0.033 |
| HClO | 1.658e-025 | 1.658e-025 | -24.780 | -24.780 | 0.000 |
| Cl(3) | 2.924e-032 | | | | |
| ClO2- | 2.924e-032 | 2.709e-032 | -31.534 | -31.567 | -0.033 |
| HClO2 | 2.360e-040 | 2.360e-040 | -39.627 | -39.627 | 0.000 |
| Cl(5) | 2.114e-028 | | | | |
| ClO3- | 2.114e-028 | 1.956e-028 | -27.675 | -27.709 | -0.034 |
| Cl(7) | 6.459e-029 | | | | |
| ClO4- | 6.459e-029 | 5.979e-029 | -28.190 | -28.223 | -0.034 |
| Fe(2) | 3.448e-028 | | | | |
| Fe(OH)3- | 2.755e-028 | 2.553e-028 | -27.560 | -27.593 | -0.033 |
| Fe(OH)2 | 3.779e-029 | 3.779e-029 | -28.423 | -28.423 | 0.000 |
| FeOH+ | 3.026e-029 | 2.803e-029 | -28.519 | -28.552 | -0.033 |
| Fe+2 | 7.010e-031 | 5.223e-031 | -30.154 | -30.282 | -0.128 |
| FeCO3 | 3.857e-031 | 3.857e-031 | -30.414 | -30.414 | 0.000 |
| Fe(OH)4-2 | 5.889e-032 | 4.332e-032 | -31.230 | -31.363 | -0.133 |
| FeSO4 | 3.647e-032 | 3.647e-032 | -31.438 | -31.438 | 0.000 |
| FeHCO3+ | 5.110e-034 | 4.734e-034 | -33.292 | -33.325 | -0.033 |
| FeCl+ | 1.374e-034 | 1.273e-034 | -33.862 | -33.895 | -0.033 |
| FeCl2 | 2.263e-040 | 2.263e-040 | -39.645 | -39.645 | 0.000 |
| FeCl4-2 | 0.000e+000 | 0.000e+000 | -45.975 | -46.108 | -0.133 |
| Fe(3) | 6.377e-011 | | | | |
| Fe(OH)4- | 6.242e-011 | 5.782e-011 | -10.205 | -10.238 | -0.033 |
| Fe(OH)3 | 1.356e-012 | 1.356e-012 | -11.868 | -11.868 | 0.000 |
| Fe(OH)2+ | 1.845e-017 | 1.709e-017 | -16.734 | -16.767 | -0.033 |
| FeOH+2 | 4.120e-025 | 3.041e-025 | -24.385 | -24.517 | -0.132 |
| FeCO3+ | 4.404e-029 | 4.080e-029 | -28.356 | -28.389 | -0.033 |
| Fe+3 | 5.179e-034 | 2.775e-034 | -33.286 | -33.557 | -0.271 |

| | | | | | |
|---|---|---|---|---|---|
| FeSO4+ | 8.906e-036 | 8.251e-036 | -35.050 | -35.084 | -0.033 |
| FeNO3+2 | 1.358e-036 | 1.002e-036 | -35.867 | -35.999 | -0.132 |
| Fe(SO4)2- | 9.512e-038 | 8.812e-038 | -37.022 | -37.055 | -0.033 |
| FeCl+2 | 1.338e-038 | 9.874e-039 | -37.874 | -38.005 | -0.132 |
| FeCl2+ | 4.883e-039 | 4.524e-039 | -38.311 | -38.344 | -0.033 |
| Fe2(OH)2+4 | 0.000e+000 | 0.000e+000 | -47.087 | -47.604 | -0.517 |
| FeNO2+2 | 0.000e+000 | 0.000e+000 | -47.333 | -47.465 | -0.132 |
| FeCl4- | 0.000e+000 | 0.000e+000 | -48.149 | -48.182 | -0.033 |
| Fe3(OH)4+5 | 0.000e+000 | 0.000e+000 | -61.251 | -62.051 | -0.800 |
| H(0) | 0.000e+000 | | | | |
| H2 | 0.000e+000 | 0.000e+000 | -45.516 | -45.515 | 0.001 |
| K | 1.356e-006 | | | | |
| K+ | 1.351e-006 | 1.249e-006 | -5.869 | -5.903 | -0.034 |
| KSO4- | 4.608e-009 | 4.269e-009 | -8.337 | -8.370 | -0.033 |
| KOH | 7.350e-010 | 7.350e-010 | -9.134 | -9.134 | 0.000 |
| KCl | 1.198e-011 | 1.198e-011 | -10.922 | -10.922 | 0.000 |
| KHSO4 | 1.557e-020 | 1.557e-020 | -19.808 | -19.808 | 0.000 |
| Li | 9.497e-014 | | | | |
| Li+ | 9.438e-014 | 8.772e-014 | -13.025 | -13.057 | -0.032 |
| LiOH | 3.410e-016 | 3.410e-016 | -15.467 | -15.467 | 0.000 |
| LiSO4- | 2.456e-016 | 2.276e-016 | -15.610 | -15.643 | -0.033 |
| LiCl | 9.349e-019 | 9.349e-019 | -18.029 | -18.029 | 0.000 |
| Mg | 4.183e-004 | | | | |
| Mg+2 | 3.885e-004 | 2.929e-004 | -3.411 | -3.533 | -0.123 |
| MgSO4 | 2.682e-005 | 2.682e-005 | -4.571 | -4.571 | 0.000 |
| MgCO3 | 2.885e-006 | 2.885e-006 | -5.540 | -5.540 | 0.000 |
| MgCl+ | 8.698e-008 | 8.058e-008 | -7.061 | -7.094 | -0.033 |
| MgHCO3+ | 6.204e-009 | 5.747e-009 | -8.207 | -8.241 | -0.033 |
| Mg4(OH)4+4 | 3.570e-009 | 1.085e-009 | -8.447 | -8.964 | -0.517 |
| N(-03) | 0.000e+000 | | | | |
| N3- | 0.000e+000 | 0.000e+000 | -107.889 | -107.922 | -0.033 |
| HN3 | 0.000e+000 | 0.000e+000 | -114.362 | -114.362 | 0.000 |
| N(-3) | 0.000e+000 | | | | |
| NH3 | 0.000e+000 | 0.000e+000 | -70.290 | -70.290 | 0.000 |
| NH4+ | 0.000e+000 | 0.000e+000 | -71.947 | -71.981 | -0.034 |
| NH4SO4- | 0.000e+000 | 0.000e+000 | -83.902 | -83.936 | -0.033 |
| N(0) | 4.302e-027 | | | | |
| N2 | 2.151e-027 | 2.151e-027 | -26.667 | -26.667 | 0.000 |
| N(3) | 9.451e-018 | | | | |
| NO2- | 9.451e-018 | 8.741e-018 | -17.025 | -17.058 | -0.034 |
| HNO2 | 1.077e-025 | 1.077e-025 | -24.968 | -24.968 | 0.000 |
| FeNO2+2 | 0.000e+000 | 0.000e+000 | -47.333 | -47.465 | -0.132 |
| N(5) | 3.911e-004 | | | | |
| NO3- | 3.905e-004 | 3.611e-004 | -3.408 | -3.442 | -0.034 |
| CaNO3+ | 6.287e-007 | 5.824e-007 | -6.202 | -6.235 | -0.033 |
| HNO3 | 8.861e-017 | 8.861e-017 | -16.053 | -16.053 | 0.000 |
| FeNO3+2 | 1.358e-036 | 1.002e-036 | -35.867 | -35.999 | -0.132 |
| Na | 2.234e-003 | | | | |
| Na+ | 2.135e-003 | 1.978e-003 | -2.671 | -2.704 | -0.033 |
| NaHSiO3 | 9.249e-005 | 9.249e-005 | -4.034 | -4.034 | 0.000 |
| NaSO4- | 6.213e-006 | 5.756e-006 | -5.207 | -5.240 | -0.033 |
| NaOH | 2.716e-007 | 2.716e-007 | -6.566 | -6.566 | 0.000 |
| NaCl | 1.124e-007 | 1.124e-007 | -6.949 | -6.949 | 0.000 |
| NaCO3- | 1.018e-007 | 9.432e-008 | -6.992 | -7.025 | -0.033 |
| NaHCO3 | 5.857e-009 | 5.857e-009 | -8.232 | -8.232 | 0.000 |
| NaAlO2 | 8.106e-010 | 8.106e-010 | -9.091 | -9.091 | 0.000 |
| O(0) | 9.210e-005 | | | | |
| O2 | 4.605e-005 | 4.611e-005 | -4.337 | -4.336 | 0.001 |
| S(-2) | 0.000e+000 | | | | |
| HS- | 0.000e+000 | 0.000e+000 | -149.158 | -149.192 | -0.034 |
| S-2 | 0.000e+000 | 0.000e+000 | -151.043 | -151.173 | -0.131 |
| H2S | 0.000e+000 | 0.000e+000 | -153.278 | -153.278 | 0.000 |

```
  S2-2              0.000e+000  0.000e+000  -265.909  -266.043    -0.133
  S3-2              0.000e+000  0.000e+000  -380.816  -380.949    -0.133
  S4-2              0.000e+000  0.000e+000  -495.954  -496.087    -0.133
  S5-2              0.000e+000  0.000e+000  -611.317  -611.450    -0.133
S(2)         0.000e+000
  S2O3-2            0.000e+000  0.000e+000  -158.769  -158.903    -0.133
  HS2O3-            0.000e+000  0.000e+000  -169.085  -169.118    -0.033
S(3)         0.000e+000
  S2O4-2            0.000e+000  0.000e+000  -145.218  -145.348    -0.131
S(4)         0.000e+000
  SO3-2             0.000e+000  0.000e+000   -49.218   -49.350    -0.132
  HSO3-             0.000e+000  0.000e+000   -53.366   -53.399    -0.033
  H2SO3             0.000e+000  0.000e+000   -62.596   -62.596     0.000
  SO2               0.000e+000  0.000e+000   -62.842   -62.842     0.000
  S2O6-2            0.000e+000  0.000e+000   -80.292   -80.426    -0.133
  S3O6-2            0.000e+000  0.000e+000  -197.726  -197.859    -0.133
  S4O6-2            0.000e+000  0.000e+000  -298.912  -299.045    -0.133
  S5O6-2            0.000e+000  0.000e+000  -429.572  -429.705    -0.133
S(5)         0.000e+000
  S2O5-2            0.000e+000  0.000e+000  -111.475  -111.608    -0.133
S(6)         6.510e-004
  SO4-2             5.989e-004  4.406e-004    -3.223    -3.356    -0.133
  MgSO4             2.682e-005  2.682e-005    -4.571    -4.571     0.000
  CaSO4             1.900e-005  1.900e-005    -4.721    -4.721     0.000
  NaSO4-            6.213e-006  5.756e-006    -5.207    -5.240    -0.033
  KSO4-             4.608e-009  4.269e-009    -8.337    -8.370    -0.033
  HSO4-             2.167e-013  2.007e-013   -12.664   -12.697    -0.033
  LiSO4-            2.456e-016  2.276e-016   -15.610   -15.643    -0.033
  KHSO4             1.557e-020  1.557e-020   -19.808   -19.808     0.000
  H2SO4             1.458e-027  1.458e-027   -26.836   -26.836     0.000
  AlSO4+            1.218e-027  1.129e-027   -26.914   -26.947    -0.033
  Al(SO4)2-         4.167e-029  3.860e-029   -28.380   -28.413    -0.033
  FeSO4             3.647e-032  3.647e-032   -31.438   -31.438     0.000
  FeSO4+            8.906e-036  8.251e-036   -35.050   -35.084    -0.033
  Fe(SO4)2-         9.512e-038  8.812e-038   -37.022   -37.055    -0.033
  NH4SO4-           0.000e+000  0.000e+000   -83.902   -83.936    -0.033
S(7)         0.000e+000
  S2O8-2            0.000e+000  0.000e+000   -54.783   -54.916    -0.133
S(8)         1.633e-035
  HSO5-             1.633e-035  1.513e-035   -34.787   -34.820    -0.033
Si           1.068e-003
  HSiO3-            8.906e-004  8.251e-004    -3.050    -3.084    -0.033
  NaHSiO3           9.249e-005  9.249e-005    -4.034    -4.034     0.000
  SiO2              5.917e-005  5.917e-005    -4.228    -4.228     0.000
  H2SiO4-2          2.540e-005  1.869e-005    -4.595    -4.728    -0.133
  H4(H2SiO4)4-4     3.991e-008  1.167e-008    -7.399    -7.933    -0.534
  H6(H2SiO4)4-2     1.099e-008  8.084e-009    -7.959    -8.092    -0.133
```

## File 28. Degraded Cement, Maximum ions, 95%/5% Mixing Ratio

*INPUT FILE*

```
SOLUTION 1
    temp      15
    pH        7.5
    pe        4
    redox     pe
    units     mmol/kgw
    density   1
    Alkalinity 0
    Cl(-1)    7.5
    Li        1e-010
```

```
    Al        1e-010
    Ca        3.1
    Mg        5
    Na        18
    K         1.9
    S(6)      7.3
    N(5)      7.9
    C(4)      21.8
    Br(-1)    0
    Si        0.01
    -water    0.144 # kg

EQUILIBRIUM_PHASES 1
    Brucite   0 1.39
    Calcite   0 9.5
    Gibbsite  0 1e-010
    Goethite  0 0.001
    SiO2(am)  0 4
    CSH(0.25) 0 12
GAS_PHASE 1
    -fixed_pressure
    -pressure 1
    -volume 1
    -temperature 25
    CO2(g)    0.056
SAVE solution 1-1
END
SOLUTION 2
    temp      25
    pH        7.5
    pe        4
    redox     pe
    units     mmol/kgs
    density   1
    Li        0
    Alkalinity 0
    Ca        3.1
    Mg        5
    Na        18
    C(4)      21.8
    Cl        7.5
    S(6)      7.3
    N(5)      7.8
    Si        0.001
    K         1.9
    -water    0.144 # kg
GAS_PHASE 2
    -fixed_pressure
    -pressure 1
    -volume 1
    -temperature 25
    CO2(g)    0.056
    O2(g)     0.18
EQUILIBRIUM_PHASES 2
    calcite   0 1
SAVE solution 2-2
END
MIX 1
    1    0.95
    2    0.05
EQUILIBRIUM_PHASES 3
    Albite    0 0.6
```

```
Calcite   0 0.1
K-Feldspar 0 0.6
Quartz    0 72
SiO2(am)  0 17.3
```

*SAMPLE OUTPUT, FINAL TIME STEP (FILE 28)*

```
------------------------------------------
Beginning of batch-reaction calculations.
------------------------------------------

Reaction step 1.

Using mix 1.
Using pure phase assemblage 3.

Mixture 1.

      9.500e-001 Solution 1       Solution after simulation 1.
      5.000e-002 Solution 2       Solution after simulation 2.

-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
Phase              SI log IAP  log KT      Initial       Final       Delta

Albite           0.00    2.93    2.93   6.000e-001  5.997e-001 -2.720e-004
Calcite          0.00    1.97    1.97   1.000e-001  1.002e-001  1.757e-004
K-Feldspar       0.00   -0.27   -0.27   6.000e-001  6.003e-001  2.719e-004
Quartz           0.00   -4.23   -4.23   7.200e+001  8.930e+001  1.730e+001
SiO2(am)        -1.36   -4.23   -2.87   1.730e+001           0 -1.730e+001

-----------------------------Solution composition------------------------------

      Elements          Molality       Moles

      Al             3.775e-007  5.440e-008
      C              7.208e-005  1.039e-005
      Ca             2.962e-004  4.268e-005
      Cl             7.496e-003  1.080e-003
      Fe             8.331e-011  1.200e-011
      K              1.177e-005  1.697e-006
      Li             9.494e-014  1.368e-014
      Mg             4.476e-004  6.450e-005
      N              7.891e-003  1.137e-003
      Na             1.988e-002  2.864e-003
      S              7.296e-003  1.051e-003
      Si             3.713e-003  5.350e-004

----------------------------Description of solution----------------------------

                                pH  =  11.545      Charge balance
                                pe  =   9.577      Adjusted to redox equilibrium
                     Activity of water  =   0.999
                        Ionic strength  =  3.382e-002
                     Mass of water (kg)  =  1.441e-001
                Total alkalinity (eq/kg)  =  5.875e-003
                     Total CO2 (mol/kg)  =  7.208e-005
                    Temperature (deg C)  =  15.500
                  Electrical balance (eq)  = -2.086e-003
Percent error, 100*(Cat-|An|)/(Cat+|An|)  = -27.49
                           Iterations  =  14
```

Total H = 1.600278e+001
Total O = 8.010535e+000

----------Distribution of species----------

| Species | Molality | Log Activity | Log Molality | Log Activity | Gamma |
|---|---|---|---|---|---|
| OH- | 1.909e-003 | 1.605e-003 | -2.719 | -2.795 | -0.075 |
| H+ | 3.268e-012 | 2.854e-012 | -11.486 | -11.545 | -0.059 |
| H2O | 5.553e+001 | 9.992e-001 | 1.744 | -0.000 | 0.000 |
| Al | 3.775e-007 | | | | |
| AlO2- | 3.767e-007 | 3.181e-007 | -6.424 | -6.497 | -0.073 |
| NaAlO2 | 8.106e-010 | 8.106e-010 | -9.091 | -9.091 | 0.000 |
| HAlO2 | 4.304e-012 | 4.304e-012 | -11.366 | -11.366 | 0.000 |
| Al(OH)2+ | 1.847e-017 | 1.560e-017 | -16.733 | -16.807 | -0.073 |
| AlOH+2 | 7.146e-023 | 3.658e-023 | -22.146 | -22.437 | -0.291 |
| AlSO4+ | 7.360e-029 | 6.215e-029 | -28.133 | -28.207 | -0.073 |
| Al+3 | 6.233e-029 | 1.796e-029 | -28.205 | -28.746 | -0.540 |
| Al(SO4)2- | 1.932e-029 | 1.631e-029 | -28.714 | -28.787 | -0.073 |
| Al2(OH)2+4 | 0.000e+000 | 0.000e+000 | -40.979 | -42.093 | -1.114 |
| Al3(OH)4+5 | 0.000e+000 | 0.000e+000 | -52.237 | -53.940 | -1.703 |
| Al13O4(OH)24+7 | 0.000e+000 | 0.000e+000 | -99.667 | -103.006 | -3.340 |
| C(-2) | 0.000e+000 | | | | |
| C2H4 | 0.000e+000 | 0.000e+000 | -284.699 | -284.699 | 0.000 |
| C(-3) | 0.000e+000 | | | | |
| C2H6 | 0.000e+000 | 0.000e+000 | -255.857 | -255.857 | 0.000 |
| C(-4) | 0.000e+000 | | | | |
| CH4 | 0.000e+000 | 0.000e+000 | -157.685 | -157.685 | 0.000 |
| C(2) | 0.000e+000 | | | | |
| CO | 0.000e+000 | 0.000e+000 | -58.311 | -58.311 | 0.000 |
| C(4) | 7.208e-005 | | | | |
| CO3-2 | 5.597e-005 | 2.865e-005 | -4.252 | -4.543 | -0.291 |
| CaCO3 | 6.353e-006 | 6.353e-006 | -5.197 | -5.197 | 0.000 |
| MgCO3 | 4.719e-006 | 4.719e-006 | -5.326 | -5.326 | 0.000 |
| HCO3- | 2.662e-006 | 2.248e-006 | -5.575 | -5.648 | -0.073 |
| NaCO3- | 2.306e-006 | 1.947e-006 | -5.637 | -5.711 | -0.073 |
| NaHCO3 | 5.855e-008 | 5.855e-008 | -7.233 | -7.233 | 0.000 |
| MgHCO3+ | 5.392e-009 | 4.553e-009 | -8.268 | -8.342 | -0.073 |
| CaHCO3+ | 3.724e-009 | 3.145e-009 | -8.429 | -8.502 | -0.073 |
| CO2 | 1.698e-011 | 1.712e-011 | -10.770 | -10.766 | 0.004 |
| FeCO3+ | 8.632e-030 | 7.288e-030 | -29.064 | -29.137 | -0.073 |
| FeCO3 | 1.381e-031 | 1.381e-031 | -30.860 | -30.860 | 0.000 |
| FeHCO3+ | 9.721e-035 | 8.208e-035 | -34.012 | -34.086 | -0.073 |
| Ca | 2.962e-004 | | | | |
| Ca+2 | 2.237e-004 | 1.197e-004 | -3.650 | -3.922 | -0.271 |
| CaSO4 | 5.426e-005 | 5.426e-005 | -4.265 | -4.265 | 0.000 |
| CaOH+ | 7.014e-006 | 5.922e-006 | -5.154 | -5.227 | -0.073 |
| CaCO3 | 6.353e-006 | 6.353e-006 | -5.197 | -5.197 | 0.000 |
| CaNO3+ | 4.691e-006 | 3.961e-006 | -5.329 | -5.402 | -0.073 |
| CaCl+ | 1.835e-007 | 1.550e-007 | -6.736 | -6.810 | -0.073 |
| CaHCO3+ | 3.724e-009 | 3.145e-009 | -8.429 | -8.502 | -0.073 |
| CaCl2 | 1.264e-009 | 1.264e-009 | -8.898 | -8.898 | 0.000 |
| Cl(-1) | 7.496e-003 | | | | |
| Cl- | 7.479e-003 | 6.260e-003 | -2.126 | -2.203 | -0.077 |
| NaCl | 1.555e-005 | 1.555e-005 | -4.808 | -4.808 | 0.000 |
| MgCl+ | 1.046e-006 | 8.832e-007 | -5.980 | -6.054 | -0.073 |
| CaCl+ | 1.835e-007 | 1.550e-007 | -6.736 | -6.810 | -0.073 |
| KCl | 1.657e-009 | 1.657e-009 | -8.781 | -8.781 | 0.000 |
| CaCl2 | 1.264e-009 | 1.264e-009 | -8.898 | -8.898 | 0.000 |
| HCl | 3.943e-015 | 3.943e-015 | -14.404 | -14.404 | 0.000 |
| LiCl | 1.521e-017 | 1.521e-017 | -16.818 | -16.818 | 0.000 |

| | | | | | |
|---|---|---|---|---|---|
| FeCl+ | 3.618e-034 | 3.055e-034 | -33.442 | -33.515 | -0.073 |
| FeCl2+ | 1.155e-037 | 9.754e-038 | -36.937 | -37.011 | -0.073 |
| FeCl+2 | 2.309e-038 | 1.182e-038 | -37.637 | -37.927 | -0.291 |
| FeCl2 | 9.777e-039 | 9.777e-039 | -38.010 | -38.010 | 0.000 |
| FeCl4-2 | 0.000e+000 | 0.000e+000 | -41.664 | -41.962 | -0.298 |
| FeCl4- | 0.000e+000 | 0.000e+000 | -44.264 | -44.338 | -0.073 |
| Cl(1) | 1.717e-020 | | | | |
| ClO- | 1.717e-020 | 1.450e-020 | -19.765 | -19.839 | -0.073 |
| HClO | 1.534e-024 | 1.534e-024 | -23.814 | -23.814 | 0.000 |
| Cl(3) | 6.505e-031 | | | | |
| ClO2- | 6.505e-031 | 5.493e-031 | -30.187 | -30.260 | -0.073 |
| HClO2 | 2.317e-039 | 2.317e-039 | -38.635 | -38.635 | 0.000 |
| Cl(5) | 5.005e-027 | | | | |
| ClO3- | 5.005e-027 | 4.208e-027 | -26.301 | -26.376 | -0.075 |
| Cl(7) | 1.623e-027 | | | | |
| ClO4- | 1.623e-027 | 1.365e-027 | -26.790 | -26.865 | -0.075 |
| Fe(2) | 3.849e-028 | | | | |
| Fe(OH)3- | 3.538e-028 | 2.987e-028 | -27.451 | -27.525 | -0.073 |
| Fe(OH)2 | 2.143e-029 | 2.143e-029 | -28.669 | -28.669 | 0.000 |
| FeOH+ | 9.124e-030 | 7.704e-030 | -29.040 | -29.113 | -0.073 |
| Fe(OH)4-2 | 2.077e-031 | 1.046e-031 | -30.683 | -30.980 | -0.298 |
| FeCO3 | 1.381e-031 | 1.381e-031 | -30.860 | -30.860 | 0.000 |
| Fe+2 | 1.300e-031 | 6.958e-032 | -30.886 | -31.158 | -0.271 |
| FeSO4 | 3.729e-032 | 3.729e-032 | -31.428 | -31.428 | 0.000 |
| FeCl+ | 3.618e-034 | 3.055e-034 | -33.442 | -33.515 | -0.073 |
| FeHCO3+ | 9.721e-035 | 8.208e-035 | -34.012 | -34.086 | -0.073 |
| FeCl2 | 9.777e-039 | 9.777e-039 | -38.010 | -38.010 | 0.000 |
| FeCl4-2 | 0.000e+000 | 0.000e+000 | -41.664 | -41.962 | -0.298 |
| Fe(3) | 8.331e-011 | | | | |
| Fe(OH)4- | 8.252e-011 | 6.968e-011 | -10.083 | -10.157 | -0.073 |
| Fe(OH)3 | 7.922e-013 | 7.922e-013 | -12.101 | -12.101 | 0.000 |
| Fe(OH)2+ | 5.728e-018 | 4.837e-018 | -17.242 | -17.315 | -0.073 |
| FeOH+2 | 8.148e-026 | 4.171e-026 | -25.089 | -25.380 | -0.291 |
| FeCO3+ | 8.632e-030 | 7.288e-030 | -29.064 | -29.137 | -0.073 |
| Fe+3 | 6.404e-035 | 1.845e-035 | -34.194 | -34.734 | -0.540 |
| FeSO4+ | 4.986e-036 | 4.210e-036 | -35.302 | -35.376 | -0.073 |
| FeNO3+2 | 2.379e-036 | 1.218e-036 | -35.624 | -35.914 | -0.291 |
| Fe(SO4)2- | 4.087e-037 | 3.451e-037 | -36.389 | -36.462 | -0.073 |
| FeCl2+ | 1.155e-037 | 9.754e-038 | -36.937 | -37.011 | -0.073 |
| FeCl+2 | 2.309e-038 | 1.182e-038 | -37.637 | -37.927 | -0.291 |
| FeCl4- | 0.000e+000 | 0.000e+000 | -44.264 | -44.338 | -0.073 |
| FeNO2+2 | 0.000e+000 | 0.000e+000 | -47.115 | -47.406 | -0.291 |
| Fe2(OH)2+4 | 0.000e+000 | 0.000e+000 | -48.215 | -49.329 | -1.114 |
| Fe3(OH)4+5 | 0.000e+000 | 0.000e+000 | -62.622 | -64.325 | -1.703 |
| H(0) | 0.000e+000 | | | | |
| H2 | 0.000e+000 | 0.000e+000 | -45.545 | -45.541 | 0.004 |
| K | 1.177e-005 | | | | |
| K+ | 1.146e-005 | 9.594e-006 | -4.941 | -5.018 | -0.077 |
| KSO4- | 2.981e-007 | 2.517e-007 | -6.526 | -6.599 | -0.073 |
| KOH | 1.165e-008 | 1.165e-008 | -7.934 | -7.934 | 0.000 |
| KCl | 1.657e-009 | 1.657e-009 | -8.781 | -8.781 | 0.000 |
| KHSO4 | 4.446e-019 | 4.446e-019 | -18.352 | -18.352 | 0.000 |
| Li | 9.494e-014 | | | | |
| Li+ | 9.242e-014 | 7.923e-014 | -13.034 | -13.101 | -0.067 |
| LiSO4- | 1.869e-015 | 1.578e-015 | -14.728 | -14.802 | -0.073 |
| LiOH | 6.356e-016 | 6.356e-016 | -15.197 | -15.197 | 0.000 |
| LiCl | 1.521e-017 | 1.521e-017 | -16.818 | -16.818 | 0.000 |
| Mg | 4.476e-004 | | | | |
| Mg+2 | 3.164e-004 | 1.782e-004 | -3.500 | -3.749 | -0.249 |
| MgSO4 | 1.253e-004 | 1.253e-004 | -3.902 | -3.902 | 0.000 |
| MgCO3 | 4.719e-006 | 4.719e-006 | -5.326 | -5.326 | 0.000 |
| MgCl+ | 1.046e-006 | 8.832e-007 | -5.980 | -6.054 | -0.073 |

| | | | | | |
|---|---|---|---|---|---|
| Mg4(OH)4+4 | 3.511e-008 | 2.699e-009 | -7.455 | -8.569 | -1.114 |
| MgHCO3+ | 5.392e-009 | 4.553e-009 | -8.268 | -8.342 | -0.073 |
| N(-03) | 0.000e+000 | | | | |
| N3- | 0.000e+000 | 0.000e+000 | -104.898 | -104.972 | -0.073 |
| HN3 | 0.000e+000 | 0.000e+000 | -111.726 | -111.726 | 0.000 |
| N(-3) | 0.000e+000 | | | | |
| NH3 | 0.000e+000 | 0.000e+000 | -69.446 | -69.446 | 0.000 |
| NH4+ | 0.000e+000 | 0.000e+000 | -71.373 | -71.452 | -0.079 |
| NH4SO4- | 0.000e+000 | 0.000e+000 | -82.448 | -82.522 | -0.073 |
| N(0) | 2.509e-025 | | | | |
| N2 | 1.254e-025 | 1.254e-025 | -24.902 | -24.902 | 0.000 |
| N(3) | 1.799e-016 | | | | |
| NO2- | 1.799e-016 | 1.506e-016 | -15.745 | -15.822 | -0.077 |
| HNO2 | 8.984e-025 | 8.984e-025 | -24.047 | -24.047 | 0.000 |
| FeNO2+2 | 0.000e+000 | 0.000e+000 | -47.115 | -47.406 | -0.291 |
| N(5) | 7.891e-003 | | | | |
| NO3- | 7.886e-003 | 6.601e-003 | -2.103 | -2.180 | -0.077 |
| CaNO3+ | 4.691e-006 | 3.961e-006 | -5.329 | -5.402 | -0.073 |
| HNO3 | 7.843e-016 | 7.843e-016 | -15.105 | -15.105 | 0.000 |
| FeNO3+2 | 2.379e-036 | 1.218e-036 | -35.624 | -35.914 | -0.291 |
| Na | 1.988e-002 | | | | |
| Na+ | 1.799e-002 | 1.519e-002 | -1.745 | -1.818 | -0.073 |
| NaHSiO3 | 1.466e-003 | 1.466e-003 | -2.834 | -2.834 | 0.000 |
| NaSO4- | 4.019e-004 | 3.394e-004 | -3.396 | -3.469 | -0.073 |
| NaCl | 1.555e-005 | 1.555e-005 | -4.808 | -4.808 | 0.000 |
| NaOH | 4.304e-006 | 4.304e-006 | -5.366 | -5.366 | 0.000 |
| NaCO3- | 2.306e-006 | 1.947e-006 | -5.637 | -5.711 | -0.073 |
| NaHCO3 | 5.855e-008 | 5.855e-008 | -7.233 | -7.233 | 0.000 |
| NaAlO2 | 8.106e-010 | 8.106e-010 | -9.091 | -9.091 | 0.000 |
| O(0) | 1.030e-004 | | | | |
| O2 | 5.148e-005 | 5.190e-005 | -4.288 | -4.285 | 0.004 |
| S(-2) | 0.000e+000 | | | | |
| HS- | 0.000e+000 | 0.000e+000 | -148.649 | -148.724 | -0.075 |
| S-2 | 0.000e+000 | 0.000e+000 | -150.107 | -150.391 | -0.284 |
| H2S | 0.000e+000 | 0.000e+000 | -153.126 | -153.126 | 0.000 |
| S2-2 | 0.000e+000 | 0.000e+000 | -264.784 | -265.082 | -0.298 |
| S3-2 | 0.000e+000 | 0.000e+000 | -379.512 | -379.810 | -0.298 |
| S4-2 | 0.000e+000 | 0.000e+000 | -494.471 | -494.769 | -0.298 |
| S5-2 | 0.000e+000 | 0.000e+000 | -609.656 | -609.954 | -0.298 |
| S(2) | 0.000e+000 | | | | |
| S2O3-2 | 0.000e+000 | 0.000e+000 | -157.567 | -157.865 | -0.298 |
| HS2O3- | 0.000e+000 | 0.000e+000 | -168.322 | -168.395 | -0.073 |
| S(3) | 0.000e+000 | | | | |
| S2O4-2 | 0.000e+000 | 0.000e+000 | -144.000 | -144.284 | -0.284 |
| S(4) | 0.000e+000 | | | | |
| SO3-2 | 0.000e+000 | 0.000e+000 | -48.200 | -48.490 | -0.291 |
| HSO3- | 0.000e+000 | 0.000e+000 | -52.781 | -52.854 | -0.073 |
| H2SO3 | 0.000e+000 | 0.000e+000 | -62.366 | -62.366 | 0.000 |
| SO2 | 0.000e+000 | 0.000e+000 | -62.612 | -62.612 | 0.000 |
| S2O6-2 | 0.000e+000 | 0.000e+000 | -79.013 | -79.310 | -0.298 |
| S3O6-2 | 0.000e+000 | 0.000e+000 | -196.267 | -196.565 | -0.298 |
| S4O6-2 | 0.000e+000 | 0.000e+000 | -297.275 | -297.573 | -0.298 |
| S5O6-2 | 0.000e+000 | 0.000e+000 | -427.757 | -428.054 | -0.298 |
| S(5) | 0.000e+000 | | | | |
| S2O5-2 | 0.000e+000 | 0.000e+000 | -110.221 | -110.519 | -0.298 |
| S(6) | 7.296e-003 | | | | |
| SO4-2 | 6.715e-003 | 3.382e-003 | -2.173 | -2.471 | -0.298 |
| NaSO4- | 4.019e-004 | 3.394e-004 | -3.396 | -3.469 | -0.073 |
| MgSO4 | 1.253e-004 | 1.253e-004 | -3.902 | -3.902 | 0.000 |
| CaSO4 | 5.426e-005 | 5.426e-005 | -4.265 | -4.265 | 0.000 |
| KSO4- | 2.981e-007 | 2.517e-007 | -6.526 | -6.599 | -0.073 |
| HSO4- | 8.837e-013 | 7.462e-013 | -12.054 | -12.127 | -0.073 |

```
   LiSO4-              1.869e-015  1.578e-015   -14.728   -14.802    -0.073
   KHSO4               4.446e-019  4.446e-019   -18.352   -18.352     0.000
   H2SO4               2.624e-027  2.624e-027   -26.581   -26.581     0.000
   AlSO4+              7.360e-029  6.215e-029   -28.133   -28.207    -0.073
   Al(SO4)2-           1.932e-029  1.631e-029   -28.714   -28.787    -0.073
   FeSO4               3.729e-032  3.729e-032   -31.428   -31.428     0.000
   FeSO4+              4.986e-036  4.210e-036   -35.302   -35.376    -0.073
   Fe(SO4)2-           4.087e-037  3.451e-037   -36.389   -36.462    -0.073
   NH4SO4-             0.000e+000  0.000e+000   -82.448   -82.522    -0.073
S(7)          0.000e+000
   S2O8-2              0.000e+000  0.000e+000   -53.452   -53.750    -0.298
S(8)          7.067e-035
   HSO5-               7.067e-035  5.967e-035   -34.151   -34.224    -0.073
Si            3.713e-003
   HSiO3-              2.016e-003  1.702e-003    -2.695    -2.769    -0.073
   NaHSiO3             1.466e-003  1.466e-003    -2.834    -2.834     0.000
   H2SiO4-2            1.580e-004  7.955e-005    -3.801    -4.099    -0.298
   SiO2                5.917e-005  5.917e-005    -4.228    -4.228     0.000
   H4(H2SiO4)4-4       3.309e-006  2.110e-007    -5.480    -6.676    -1.196
   H6(H2SiO4)4-2       6.805e-008  3.427e-008    -7.167    -7.465    -0.298
```

## File 29. Degraded Cement, Minimum ions, 50%/50% Mixing Ratio

*INPUT FILE*

```
SOLUTION 1
   temp      15
   pH        7.5 charge
   pe        4
   redox     pe
   units     mmol/kgw
   density   1
   Alkalinity 0
   Cl(-1)    0
   Li        1e-010
   Al        1e-010
   Ca        0.6
   Mg        0.3
   Na        1.3
   K         0
   S(6)      0.3
   N(5)      0
   C(4)      1.4
   Br(-1)    0
   Si        0.01
   -water    0.144 # kg

EQUILIBRIUM_PHASES 1
   Brucite   0 1.39
   Calcite   0 9.5
   Gibbsite  0 1e-010
   Goethite  0 0.001
   SiO2(am)  0 4
   CSH(0.25) 0 12
GAS_PHASE 1
   -fixed_pressure
   -pressure 1
   -volume 1
   -temperature 25
   CO2(g)    0.056
SAVE solution 1-1
END
```

```
SOLUTION 2
   temp      25
   pH        7.5 charge
   pe        4
   redox     pe
   units     mmol/kgs
   density   1
   Li        0
   Alkalinity 0
   Ca        3.1
   Mg        5
   Na        18
   C(4)      21.8
   Cl        7.5
   S(6)      7.3
   N(5)      7.8
   Si        0.001
   K         1.9
   -water    0.144 # kg
GAS_PHASE 2
   -fixed_pressure
   -pressure 1
   -volume 1
   -temperature 25
   CO2(g)    0.056
   O2(g)     0.18
EQUILIBRIUM_PHASES 2
   calcite   0 1
SAVE solution 2-2
END
MIX 1
   1    0.5
   2    0.5
EQUILIBRIUM_PHASES 3
   Albite    0 0.6
   Calcite   0 0.1
   K-Feldspar 0 0.6
   Quartz    0 72
   SiO2(am)  0 17.3
```

*SAMPLE OUTPUT, FINAL TIME STEP (FILE 29)*

```
------------------------------------------
Beginning of batch-reaction calculations.
------------------------------------------

Reaction step 1.

Using mix 1.
Using pure phase assemblage 3.

Mixture 1.

       5.000e-001 Solution 1       Solution after simulation 1.
       5.000e-001 Solution 2       Solution after simulation 2.

-------------------------------Phase assemblage--------------------------------

                                                Moles in assemblage
Phase               SI log IAP  log KT      Initial       Final       Delta

Albite            -0.00    2.80    2.80   6.000e-001  5.999e-001 -1.364e-004
```

| | | | | | | |
|---|---|---|---|---|---|---|
| Calcite | 0.00 | 1.90 | 1.90 | 1.000e-001 | 1.000e-001 | -1.717e-006 |
| K-Feldspar | -0.00 | -0.32 | -0.32 | 6.000e-001 | 6.001e-001 | 1.361e-004 |
| Quartz | 0.00 | -4.13 | -4.13 | 7.200e+001 | 8.930e+001 | 1.730e+001 |
| SiO2(am) | -1.32 | -4.13 | -2.81 | 1.730e+001 | 0 | -1.730e+001 |

----------Solution composition----------

| Elements | Molality | Moles |
|---|---|---|
| Al | 2.210e-006 | 3.183e-007 |
| C | 1.133e-002 | 1.632e-003 |
| Ca | 4.022e-003 | 5.792e-004 |
| Cl | 3.761e-003 | 5.417e-004 |
| Fe | 3.357e-011 | 4.835e-012 |
| K | 8.043e-006 | 1.158e-006 |
| Li | 4.999e-014 | 7.200e-015 |
| Mg | 2.596e-003 | 3.738e-004 |
| N | 3.912e-003 | 5.634e-004 |
| Na | 1.062e-002 | 1.530e-003 |
| S | 3.811e-003 | 5.489e-004 |
| Si | 7.422e-005 | 1.069e-005 |

----------Description of solution----------

pH = 6.790 Charge balance
pe = 14.235 Adjusted to redox equilibrium
Activity of water = 0.999
Ionic strength = 3.007e-002
Mass of water (kg) = 1.440e-001
Total alkalinity (eq/kg) = 8.578e-003
Total CO2 (mol/kg) = 1.133e-002
Temperature (deg C) = 20.000
Electrical balance (eq) = 1.059e-012
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 0.00
Iterations = 27
Total H = 1.599436e+001
Total O = 8.005101e+000

----------Distribution of species----------

| Species | Molality | Log Activity | Log Molality | Log Activity | Gamma |
|---|---|---|---|---|---|
| H+ | 1.847e-007 | 1.620e-007 | -6.733 | -6.790 | -0.057 |
| OH- | 4.784e-008 | 4.051e-008 | -7.320 | -7.392 | -0.072 |
| H2O | 5.553e+001 | 9.993e-001 | 1.744 | -0.000 | 0.000 |
| Al | 2.210e-006 | | | | |
| AlO2- | 7.740e-007 | 6.579e-007 | -6.111 | -6.182 | -0.071 |
| HAlO2 | 3.993e-007 | 3.993e-007 | -6.399 | -6.399 | 0.000 |
| Al13O4(OH)24+7 | 7.324e-008 | 4.451e-011 | -7.135 | -10.352 | -3.216 |
| Al(OH)2+ | 7.190e-008 | 6.112e-008 | -7.143 | -7.214 | -0.071 |
| AlOH+2 | 1.134e-008 | 5.962e-009 | -7.945 | -8.225 | -0.279 |
| NaAlO2 | 1.039e-009 | 1.039e-009 | -8.983 | -8.983 | 0.000 |
| Al+3 | 4.046e-010 | 1.213e-010 | -9.393 | -9.916 | -0.523 |
| AlSO4+ | 2.193e-010 | 1.864e-010 | -9.659 | -9.729 | -0.071 |
| Al(SO4)2- | 2.556e-011 | 2.173e-011 | -10.592 | -10.663 | -0.071 |
| Al2(OH)2+4 | 1.350e-013 | 1.143e-014 | -12.870 | -13.942 | -1.072 |
| Al3(OH)4+5 | 1.488e-015 | 3.407e-017 | -14.827 | -16.468 | -1.640 |
| C(-2) | 0.000e+000 | | | | |
| C2H4 | 0.000e+000 | 0.000e+000 | -266.855 | -266.855 | 0.000 |
| C(-3) | 0.000e+000 | | | | |
| C2H6 | 0.000e+000 | 0.000e+000 | -238.879 | -238.879 | 0.000 |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(-4) | 0.000e+000 | | | | | |
| CH4 | | 0.000e+000 | 0.000e+000 | -148.953 | -148.953 | 0.000 |
| C(2) | 0.000e+000 | | | | | |
| CO | | 0.000e+000 | 0.000e+000 | -49.781 | -49.781 | 0.000 |
| C(4) | 1.133e-002 | | | | | |
| HCO3- | | 8.162e-003 | 6.938e-003 | -2.088 | -2.159 | -0.071 |
| CO2 | | 2.773e-003 | 2.794e-003 | -2.557 | -2.554 | 0.003 |
| CaHCO3+ | | 1.787e-004 | 1.519e-004 | -3.748 | -3.818 | -0.071 |
| MgHCO3+ | | 1.107e-004 | 9.412e-005 | -3.956 | -4.026 | -0.071 |
| NaHCO3 | | 9.661e-005 | 9.661e-005 | -4.015 | -4.015 | 0.000 |
| CaCO3 | | 6.614e-006 | 6.614e-006 | -5.180 | -5.180 | 0.000 |
| CO3-2 | | 3.268e-006 | 1.718e-006 | -5.486 | -5.765 | -0.279 |
| MgCO3 | | 2.007e-006 | 2.007e-006 | -5.697 | -5.697 | 0.000 |
| NaCO3- | | 7.155e-008 | 6.082e-008 | -7.145 | -7.216 | -0.071 |
| FeCO3+ | | 1.847e-015 | 1.570e-015 | -14.733 | -14.804 | -0.071 |
| FeHCO3+ | | 3.098e-020 | 2.634e-020 | -19.509 | -19.579 | -0.071 |
| FeCO3 | | 7.803e-022 | 7.803e-022 | -21.108 | -21.108 | 0.000 |
| Ca | 4.022e-003 | | | | | |
| Ca+2 | | 3.407e-003 | 1.866e-003 | -2.468 | -2.729 | -0.261 |
| CaSO4 | | 3.915e-004 | 3.915e-004 | -3.407 | -3.407 | 0.000 |
| CaHCO3+ | | 1.787e-004 | 1.519e-004 | -3.748 | -3.818 | -0.071 |
| CaNO3+ | | 3.596e-005 | 3.057e-005 | -4.444 | -4.515 | -0.071 |
| CaCO3 | | 6.614e-006 | 6.614e-006 | -5.180 | -5.180 | 0.000 |
| CaCl+ | | 1.450e-006 | 1.233e-006 | -5.839 | -5.909 | -0.071 |
| CaCl2 | | 4.833e-009 | 4.833e-009 | -8.316 | -8.316 | 0.000 |
| CaOH+ | | 1.913e-009 | 1.626e-009 | -8.718 | -8.789 | -0.071 |
| Cl(-1) | 3.761e-003 | | | | | |
| Cl- | | 3.752e-003 | 3.164e-003 | -2.426 | -2.500 | -0.074 |
| NaCl | | 4.743e-006 | 4.743e-006 | -5.324 | -5.324 | 0.000 |
| MgCl+ | | 3.457e-006 | 2.938e-006 | -5.461 | -5.532 | -0.071 |
| CaCl+ | | 1.450e-006 | 1.233e-006 | -5.839 | -5.909 | -0.071 |
| CaCl2 | | 4.833e-009 | 4.833e-009 | -8.316 | -8.316 | 0.000 |
| KCl | | 6.434e-010 | 6.434e-010 | -9.192 | -9.192 | 0.000 |
| HCl | | 1.143e-010 | 1.143e-010 | -9.942 | -9.942 | 0.000 |
| LiCl | | 4.278e-018 | 4.278e-018 | -17.369 | -17.369 | 0.000 |
| FeCl2+ | | 1.611e-022 | 1.370e-022 | -21.793 | -21.863 | -0.071 |
| FeCl+2 | | 7.888e-023 | 4.147e-023 | -22.103 | -22.382 | -0.279 |
| FeCl+ | | 1.919e-023 | 1.631e-023 | -22.717 | -22.787 | -0.071 |
| FeCl2 | | 2.698e-028 | 2.698e-028 | -27.569 | -27.569 | 0.000 |
| FeCl4- | | 1.939e-030 | 1.648e-030 | -29.712 | -29.783 | -0.071 |
| FeCl4-2 | | 1.486e-032 | 7.694e-033 | -31.828 | -32.114 | -0.286 |
| Cl(1) | 2.410e-019 | | | | | |
| HClO | | 2.015e-019 | 2.015e-019 | -18.696 | -18.696 | 0.000 |
| ClO- | | 3.946e-020 | 3.354e-020 | -19.404 | -19.474 | -0.071 |
| Cl(3) | 6.060e-030 | | | | | |
| ClO2- | | 6.059e-030 | 5.150e-030 | -29.218 | -29.288 | -0.071 |
| HClO2 | | 1.234e-033 | 1.234e-033 | -32.909 | -32.909 | 0.000 |
| Cl(5) | 1.142e-025 | | | | | |
| ClO3- | | 1.142e-025 | 9.667e-026 | -24.942 | -25.015 | -0.072 |
| Cl(7) | 9.822e-026 | | | | | |
| ClO4- | | 9.822e-026 | 8.317e-026 | -25.008 | -25.080 | -0.072 |
| Fe(2) | 4.673e-020 | | | | | |
| FeHCO3+ | | 3.098e-020 | 2.634e-020 | -19.509 | -19.579 | -0.071 |
| Fe+2 | | 1.321e-020 | 7.233e-021 | -19.879 | -20.141 | -0.261 |
| FeSO4 | | 1.721e-021 | 1.721e-021 | -20.764 | -20.764 | 0.000 |
| FeCO3 | | 7.803e-022 | 7.803e-022 | -21.108 | -21.108 | 0.000 |
| FeCl+ | | 1.919e-023 | 1.631e-023 | -22.717 | -22.787 | -0.071 |
| FeOH+ | | 1.660e-023 | 1.411e-023 | -22.780 | -22.850 | -0.071 |
| Fe(OH)2 | | 6.913e-028 | 6.913e-028 | -27.160 | -27.160 | 0.000 |
| FeCl2 | | 2.698e-028 | 2.698e-028 | -27.569 | -27.569 | 0.000 |
| Fe(OH)3- | | 1.997e-031 | 1.698e-031 | -30.700 | -30.770 | -0.071 |
| FeCl4-2 | | 1.486e-032 | 7.694e-033 | -31.828 | -32.114 | -0.286 |

| | | | | | |
|---|---|---|---|---|---|
| Fe(OH)4-2 | 2.022e-039 | 1.047e-039 | -38.694 | -38.980 | -0.286 |
| Fe(3) | 3.357e-011 | | | | |
| Fe(OH)3 | 2.381e-011 | 2.381e-011 | -10.623 | -10.623 | 0.000 |
| Fe(OH)2+ | 9.708e-012 | 8.252e-012 | -11.013 | -11.083 | -0.071 |
| Fe(OH)4- | 4.340e-014 | 3.689e-014 | -13.363 | -13.433 | -0.071 |
| FeOH+2 | 7.686e-015 | 4.040e-015 | -14.114 | -14.394 | -0.279 |
| FeCO3+ | 1.847e-015 | 1.570e-015 | -14.733 | -14.804 | -0.071 |
| Fe+3 | 3.383e-019 | 1.014e-019 | -18.471 | -18.994 | -0.523 |
| FeSO4+ | 1.433e-020 | 1.218e-020 | -19.844 | -19.914 | -0.071 |
| FeNO3+2 | 6.308e-021 | 3.316e-021 | -20.200 | -20.479 | -0.279 |
| Fe(SO4)2- | 4.401e-022 | 3.742e-022 | -21.356 | -21.427 | -0.071 |
| FeCl2+ | 1.611e-022 | 1.370e-022 | -21.793 | -21.863 | -0.071 |
| FeCl+2 | 7.888e-023 | 4.147e-023 | -22.103 | -22.382 | -0.279 |
| Fe2(OH)2+4 | 5.188e-027 | 4.394e-028 | -26.285 | -27.357 | -1.072 |
| FeCl4- | 1.939e-030 | 1.648e-030 | -29.712 | -29.783 | -0.071 |
| FeNO2+2 | 1.251e-032 | 6.579e-033 | -31.903 | -32.182 | -0.279 |
| Fe3(OH)4+5 | 3.310e-035 | 7.576e-037 | -34.480 | -36.121 | -1.640 |
| H(0) | 0.000e+000 | | | | |
| H2 | 0.000e+000 | 0.000e+000 | -45.257 | -45.254 | 0.003 |
| K | 8.043e-006 | | | | |
| K+ | 7.949e-006 | 6.703e-006 | -5.100 | -5.174 | -0.074 |
| KSO4- | 9.350e-008 | 7.949e-008 | -7.029 | -7.100 | -0.071 |
| KCl | 6.434e-010 | 6.434e-010 | -9.192 | -9.192 | 0.000 |
| KOH | 1.434e-013 | 1.434e-013 | -12.844 | -12.844 | 0.000 |
| KHSO4 | 9.438e-015 | 9.438e-015 | -14.025 | -14.025 | 0.000 |
| Li | 4.999e-014 | | | | |
| Li+ | 4.955e-014 | 4.271e-014 | -13.305 | -13.369 | -0.064 |
| LiSO4- | 4.443e-016 | 3.777e-016 | -15.352 | -15.423 | -0.071 |
| LiCl | 4.278e-018 | 4.278e-018 | -17.369 | -17.369 | 0.000 |
| LiOH | 6.036e-021 | 6.036e-021 | -20.219 | -20.219 | 0.000 |
| Mg | 2.596e-003 | | | | |
| Mg+2 | 2.063e-003 | 1.185e-003 | -2.685 | -2.926 | -0.241 |
| MgSO4 | 4.165e-004 | 4.165e-004 | -3.380 | -3.380 | 0.000 |
| MgHCO3+ | 1.107e-004 | 9.412e-005 | -3.956 | -4.026 | -0.071 |
| MgCl+ | 3.457e-006 | 2.938e-006 | -5.461 | -5.532 | -0.071 |
| MgCO3 | 2.007e-006 | 2.007e-006 | -5.697 | -5.697 | 0.000 |
| Mg4(OH)4+4 | 5.989e-024 | 5.072e-025 | -23.223 | -24.295 | -1.072 |
| N(-03) | 0.000e+000 | | | | |
| N3- | 0.000e+000 | 0.000e+000 | -98.566 | -98.636 | -0.071 |
| HN3 | 0.000e+000 | 0.000e+000 | -100.679 | -100.679 | 0.000 |
| N(-3) | 0.000e+000 | | | | |
| NH4+ | 0.000e+000 | 0.000e+000 | -63.152 | -63.227 | -0.076 |
| NH3 | 0.000e+000 | 0.000e+000 | -65.832 | -65.832 | 0.000 |
| NH4SO4- | 0.000e+000 | 0.000e+000 | -74.435 | -74.506 | -0.071 |
| N(0) | 1.407e-018 | | | | |
| N2 | 7.036e-019 | 7.036e-019 | -18.153 | -18.153 | 0.000 |
| N(3) | 5.445e-017 | | | | |
| NO2- | 5.444e-017 | 4.591e-017 | -16.264 | -16.338 | -0.074 |
| HNO2 | 1.409e-020 | 1.409e-020 | -19.851 | -19.851 | 0.000 |
| FeNO2+2 | 1.251e-032 | 6.579e-033 | -31.903 | -32.182 | -0.279 |
| N(5) | 3.912e-003 | | | | |
| NO3- | 3.876e-003 | 3.268e-003 | -2.412 | -2.486 | -0.074 |
| CaNO3+ | 3.596e-005 | 3.057e-005 | -4.444 | -4.515 | -0.071 |
| HNO3 | 2.459e-011 | 2.459e-011 | -10.609 | -10.609 | 0.000 |
| FeNO3+2 | 6.308e-021 | 3.316e-021 | -20.200 | -20.479 | -0.279 |
| Na | 1.062e-002 | | | | |
| Na+ | 1.042e-002 | 8.857e-003 | -1.982 | -2.053 | -0.071 |
| NaSO4- | 1.034e-004 | 8.787e-005 | -3.986 | -4.056 | -0.071 |
| NaHCO3 | 9.661e-005 | 9.661e-005 | -4.015 | -4.015 | 0.000 |
| NaCl | 4.743e-006 | 4.743e-006 | -5.324 | -5.324 | 0.000 |
| NaCO3- | 7.155e-008 | 6.082e-008 | -7.145 | -7.216 | -0.071 |
| NaHSiO3 | 2.021e-008 | 2.021e-008 | -7.695 | -7.695 | 0.000 |

```
  NaAlO2            1.039e-009  1.039e-009   -8.983   -8.983    0.000
  NaOH              6.258e-011  6.258e-011  -10.204  -10.204    0.000
O(0)        9.211e-004
  O2            4.606e-004  4.639e-004   -3.337   -3.334    0.003
S(-2)       0.000e+000
  H2S           0.000e+000  0.000e+000  -143.535  -143.535    0.000
  HS-           0.000e+000  0.000e+000  -143.750  -143.822   -0.072
  S-2           0.000e+000  0.000e+000  -149.832  -150.105   -0.273
  S2-2          0.000e+000  0.000e+000  -255.118  -255.404   -0.286
  S3-2          0.000e+000  0.000e+000  -360.456  -360.741   -0.286
  S4-2          0.000e+000  0.000e+000  -466.023  -466.309   -0.286
  S5-2          0.000e+000  0.000e+000  -571.812  -572.098   -0.286
S(2)        0.000e+000
  S2O3-2        0.000e+000  0.000e+000  -148.307  -148.593   -0.286
  HS2O3-        0.000e+000  0.000e+000  -154.299  -154.369   -0.071
S(3)        0.000e+000
  S2O4-2        0.000e+000  0.000e+000  -134.579  -134.852   -0.273
S(4)        0.000e+000
  HSO3-         0.000e+000  0.000e+000   -48.091   -48.161   -0.071
  SO3-2         0.000e+000  0.000e+000   -48.296   -48.575   -0.279
  H2SO3         0.000e+000  0.000e+000   -52.943   -52.943    0.000
  SO2           0.000e+000  0.000e+000   -53.121   -53.121    0.000
  S2O6-2        0.000e+000  0.000e+000   -69.710   -69.996   -0.286
  S3O6-2        0.000e+000  0.000e+000  -177.553  -177.839   -0.286
  S4O6-2        0.000e+000  0.000e+000  -269.315  -269.600   -0.286
  S5O6-2        0.000e+000  0.000e+000  -390.262  -390.548   -0.286
S(5)        0.000e+000
  S2O5-2        0.000e+000  0.000e+000  -100.856  -101.142   -0.286
S(6)        3.811e-003
  SO4-2         2.900e-003  1.502e-003   -2.538   -2.823   -0.286
  MgSO4         4.165e-004  4.165e-004   -3.380   -3.380    0.000
  CaSO4         3.915e-004  3.915e-004   -3.407   -3.407    0.000
  NaSO4-        1.034e-004  8.787e-005   -3.986   -4.056   -0.071
  KSO4-         9.350e-008  7.949e-008   -7.029   -7.100   -0.071
  HSO4-         2.510e-008  2.134e-008   -7.600   -7.671   -0.071
  AlSO4+        2.193e-010  1.864e-010   -9.659   -9.729   -0.071
  Al(SO4)2-     2.556e-011  2.173e-011  -10.592  -10.663   -0.071
  KHSO4         9.438e-015  9.438e-015  -14.025  -14.025    0.000
  LiSO4-        4.443e-016  3.777e-016  -15.352  -15.423   -0.071
  H2SO4         3.756e-018  3.756e-018  -17.425  -17.425    0.000
  FeSO4+        1.433e-020  1.218e-020  -19.844  -19.914   -0.071
  FeSO4         1.721e-021  1.721e-021  -20.764  -20.764    0.000
  Fe(SO4)2-     4.401e-022  3.742e-022  -21.356  -21.427   -0.071
  NH4SO4-       0.000e+000  0.000e+000  -74.435  -74.506   -0.071
S(7)        0.000e+000
  S2O8-2        0.000e+000  0.000e+000  -43.646  -43.932   -0.286
S(8)        1.290e-029
  HSO5-         1.290e-029  1.097e-029  -28.889  -28.960   -0.071
Si          7.422e-005
  SiO2          7.415e-005  7.415e-005   -4.130   -4.130    0.000
  HSiO3-        5.174e-008  4.399e-008   -7.286   -7.357   -0.071
  NaHSiO3       2.021e-008  2.021e-008   -7.695   -7.695    0.000
  H2SiO4-2      5.974e-014  3.093e-014  -13.224  -13.510   -0.286
  H6(H2SiO4)4-2 5.068e-017  2.625e-017  -16.295  -16.581   -0.286
  H4(H2SiO4)4-4 7.027e-025  5.012e-026  -24.153  -25.300   -1.147
```

## File 30. Degraded Cement, Maximum ions, 50%/50% Mixing Ratio

*INPUT FILE*

```
SOLUTION 1
   temp      15
```

```
    pH       7.5 charge
    pe       4
    redox    pe
    units    mmol/kgw
    density  1
    Alkalinity 0
    Cl(-1)   7.5
    Li       1e-010
    Al       1e-010
    Ca       3.1
    Mg       5
    Na       18
    K        1.9
    S(6)     7.3
    N(5)     7.9
    C(4)     21.8
    Br(-1)   0
    Si       0.01
    -water   0.144 # kg

EQUILIBRIUM_PHASES 1
    Brucite   0 1.39
    Calcite   0 9.5
    Gibbsite  0 1e-010
    Goethite  0 0.001
    SiO2(am)  0 4
    CSH(0.25) 0 12
GAS_PHASE 1
    -fixed_pressure
    -pressure 1
    -volume 1
    -temperature 25
    CO2(g)    0.056
SAVE solution 1-1
END
SOLUTION 2
    temp     25
    pH       7.5 charge
    pe       4
    redox    pe
    units    mmol/kgs
    density  1
    Li       0
    Alkalinity 0
    Ca       3.1
    Mg       5
    Na       18
    C(4)     21.8
    Cl       7.5
    S(6)     7.3
    N(5)     7.8
    Si       0.001
    K        1.9
    -water   0.144 # kg
GAS_PHASE 2
    -fixed_pressure
    -pressure 1
    -volume 1
    -temperature 25
    CO2(g)   0.056
    O2(g)    0.18
EQUILIBRIUM_PHASES 2
```

```
   calcite   0 1
SAVE solution 2-2
END
MIX 1
   1    0.5
   2    0.5
EQUILIBRIUM_PHASES 3
   Albite    0 0.6
   Calcite   0 0.1
   K-Feldspar 0 0.6
   Quartz    0 72
   SiO2(am)  0 17.3
```

*SAMPLE OUTPUT, FINAL TIME STEP (FILE 30)*

```
------------------------------------------
Beginning of batch-reaction calculations.
------------------------------------------

Reaction step 1.

Using mix 1.
Using pure phase assemblage 3.

Mixture 1.

      5.000e-001 Solution 1       Solution after simulation 1.
      5.000e-001 Solution 2       Solution after simulation 2.

-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
Phase               SI log IAP  log KT      Initial       Final       Delta

Albite            -0.00    2.80    2.80   6.000e-001  5.997e-001 -2.720e-004
Calcite            0.00    1.90    1.90   1.000e-001  1.000e-001  3.196e-005
K-Feldspar        -0.00   -0.32   -0.32   6.000e-001  6.003e-001  2.718e-004
Quartz             0.00   -4.13   -4.13   7.200e+001  8.930e+001  1.730e+001
SiO2(am)          -1.32   -4.13   -2.81   1.730e+001           0 -1.730e+001

-----------------------------Solution composition------------------------------

      Elements          Molality       Moles

      Al             8.315e-007  1.198e-007
      C              1.110e-002  1.598e-003
      Ca             6.164e-003  8.879e-004
      Cl             7.509e-003  1.082e-003
      Fe             2.385e-011  3.435e-012
      K              1.516e-005  2.183e-006
      Li             4.998e-014  7.200e-015
      Mg             2.925e-003  4.214e-004
      N              7.860e-003  1.132e-003
      Na             1.991e-002  2.868e-003
      S              7.309e-003  1.053e-003
      Si             7.423e-005  1.069e-005

----------------------------Description of solution----------------------------

                                  pH  =   6.713     Charge balance
                                  pe  =  14.312     Adjusted to redox equilibrium
                        Activity of water  =   0.999
```

Ionic strength = 4.673e-002
Mass of water (kg) = 1.440e-001
Total alkalinity (eq/kg) = 8.120e-003
Total CO2 (mol/kg) = 1.110e-002
Temperature (deg C) = 20.000
Electrical balance (eq) = 1.120e-012
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 0.00
Iterations = 13
Total H = 1.599744e+001
Total O = 8.010261e+000

----------Distribution of species----------

| Species | Molality | Log Activity | Log Molality | Log Activity | Gamma |
|---|---|---|---|---|---|
| H+ | 2.248e-007 | 1.935e-007 | -6.648 | -6.713 | -0.065 |
| OH- | 4.134e-008 | 3.391e-008 | -7.384 | -7.470 | -0.086 |
| H2O | 5.553e+001 | 9.990e-001 | 1.744 | -0.000 | 0.000 |
| Al | 8.315e-007 | | | | |
| AlO2- | 4.412e-007 | 3.639e-007 | -6.355 | -6.439 | -0.084 |
| HAlO2 | 2.637e-007 | 2.637e-007 | -6.579 | -6.579 | 0.000 |
| Al(OH)2+ | 5.846e-008 | 4.821e-008 | -7.233 | -7.317 | -0.084 |
| AlOH+2 | 1.204e-008 | 5.618e-009 | -7.919 | -8.250 | -0.331 |
| Al13O4(OH)24+7 | 4.155e-009 | 7.024e-013 | -8.381 | -12.153 | -3.772 |
| NaAlO2 | 1.039e-009 | 1.039e-009 | -8.983 | -8.983 | 0.000 |
| Al+3 | 5.455e-010 | 1.366e-010 | -9.263 | -9.864 | -0.601 |
| AlSO4+ | 4.233e-010 | 3.491e-010 | -9.373 | -9.457 | -0.084 |
| Al(SO4)2- | 8.205e-011 | 6.768e-011 | -10.086 | -10.170 | -0.084 |
| Al2(OH)2+4 | 1.856e-013 | 1.015e-014 | -12.732 | -13.993 | -1.262 |
| Al3(OH)4+5 | 2.002e-015 | 2.387e-017 | -14.699 | -16.622 | -1.924 |
| C(-2) | 0.000e+000 | | | | |
| C2H4 | 0.000e+000 | 0.000e+000 | -266.792 | -266.792 | 0.000 |
| C(-3) | 0.000e+000 | | | | |
| C2H6 | 0.000e+000 | 0.000e+000 | -238.816 | -238.816 | 0.000 |
| C(-4) | 0.000e+000 | | | | |
| CH4 | 0.000e+000 | 0.000e+000 | -148.922 | -148.922 | 0.000 |
| C(2) | 0.000e+000 | | | | |
| CO | 0.000e+000 | 0.000e+000 | -49.747 | -49.747 | 0.000 |
| C(4) | 1.110e-002 | | | | |
| HCO3- | 7.618e-003 | 6.284e-003 | -2.118 | -2.202 | -0.084 |
| CO2 | 2.989e-003 | 3.023e-003 | -2.524 | -2.520 | 0.005 |
| CaHCO3+ | 2.199e-004 | 1.814e-004 | -3.658 | -3.741 | -0.084 |
| NaHCO3 | 1.582e-004 | 1.582e-004 | -3.801 | -3.801 | 0.000 |
| MgHCO3+ | 9.903e-005 | 8.168e-005 | -4.004 | -4.088 | -0.084 |
| CaCO3 | 6.614e-006 | 6.614e-006 | -5.180 | -5.180 | 0.000 |
| CO3-2 | 2.792e-006 | 1.303e-006 | -5.554 | -5.885 | -0.331 |
| MgCO3 | 1.459e-006 | 1.459e-006 | -5.836 | -5.836 | 0.000 |
| NaCO3- | 1.011e-007 | 8.339e-008 | -6.995 | -7.079 | -0.084 |
| FeCO3+ | 1.639e-015 | 1.352e-015 | -14.785 | -14.869 | -0.084 |
| FeHCO3+ | 2.746e-020 | 2.265e-020 | -19.561 | -19.645 | -0.084 |
| FeCO3 | 5.619e-022 | 5.619e-022 | -21.250 | -21.250 | 0.000 |
| Ca | 6.164e-003 | | | | |
| Ca+2 | 4.981e-003 | 2.461e-003 | -2.303 | -2.609 | -0.306 |
| CaSO4 | 8.586e-004 | 8.586e-004 | -3.066 | -3.066 | 0.000 |
| CaHCO3+ | 2.199e-004 | 1.814e-004 | -3.658 | -3.741 | -0.084 |
| CaNO3+ | 9.468e-005 | 7.809e-005 | -4.024 | -4.107 | -0.084 |
| CaCO3 | 6.614e-006 | 6.614e-006 | -5.180 | -5.180 | 0.000 |
| CaCl+ | 3.801e-006 | 3.135e-006 | -5.420 | -5.504 | -0.084 |
| CaCl2 | 2.370e-008 | 2.370e-008 | -7.625 | -7.625 | 0.000 |
| CaOH+ | 2.176e-009 | 1.795e-009 | -8.662 | -8.746 | -0.084 |
| Cl(-1) | 7.509e-003 | | | | |

| | | | | | |
|---|---|---|---|---|---|
| Cl- | 7.483e-003 | 6.101e-003 | -2.126 | -2.215 | -0.089 |
| NaCl | 1.654e-005 | 1.654e-005 | -4.782 | -4.782 | 0.000 |
| MgCl+ | 6.583e-006 | 5.430e-006 | -5.182 | -5.265 | -0.084 |
| CaCl+ | 3.801e-006 | 3.135e-006 | -5.420 | -5.504 | -0.084 |
| CaCl2 | 2.370e-008 | 2.370e-008 | -7.625 | -7.625 | 0.000 |
| KCl | 2.243e-009 | 2.243e-009 | -8.649 | -8.649 | 0.000 |
| HCl | 2.633e-010 | 2.633e-010 | -9.580 | -9.580 | 0.000 |
| LiCl | 7.999e-018 | 7.999e-018 | -17.097 | -17.097 | 0.000 |
| FeCl2+ | 7.012e-022 | 5.783e-022 | -21.154 | -21.238 | -0.084 |
| FeCl+2 | 1.946e-022 | 9.078e-023 | -21.711 | -22.042 | -0.331 |
| FeCl+ | 3.622e-023 | 2.987e-023 | -22.441 | -22.525 | -0.084 |
| FeCl2 | 9.528e-028 | 9.528e-028 | -27.021 | -27.021 | 0.000 |
| FeCl4- | 3.138e-029 | 2.588e-029 | -28.503 | -28.587 | -0.084 |
| FeCl4-2 | 2.211e-031 | 1.010e-031 | -30.655 | -30.996 | -0.340 |
| Cl(1) | 5.436e-019 | | | | |
| HClO | 4.650e-019 | 4.650e-019 | -18.333 | -18.333 | 0.000 |
| ClO- | 7.857e-020 | 6.481e-020 | -19.105 | -19.188 | -0.084 |
| Cl(3) | 1.209e-029 | | | | |
| ClO2- | 1.209e-029 | 9.970e-030 | -28.918 | -29.001 | -0.084 |
| HClO2 | 2.852e-033 | 2.852e-033 | -32.545 | -32.545 | 0.000 |
| Cl(5) | 2.286e-025 | | | | |
| ClO3- | 2.286e-025 | 1.875e-025 | -24.641 | -24.727 | -0.086 |
| Cl(7) | 1.970e-025 | | | | |
| ClO4- | 1.970e-025 | 1.616e-025 | -24.705 | -24.792 | -0.086 |
| Fe(2) | 4.469e-020 | | | | |
| FeHCO3+ | 2.746e-020 | 2.265e-020 | -19.561 | -19.645 | -0.084 |
| Fe+2 | 1.390e-020 | 6.869e-021 | -19.857 | -20.163 | -0.306 |
| FeSO4 | 2.718e-021 | 2.718e-021 | -20.566 | -20.566 | 0.000 |
| FeCO3 | 5.619e-022 | 5.619e-022 | -21.250 | -21.250 | 0.000 |
| FeCl+ | 3.622e-023 | 2.987e-023 | -22.441 | -22.525 | -0.084 |
| FeOH+ | 1.360e-023 | 1.121e-023 | -22.867 | -22.950 | -0.084 |
| FeCl2 | 9.528e-028 | 9.528e-028 | -27.021 | -27.021 | 0.000 |
| Fe(OH)2 | 4.599e-028 | 4.599e-028 | -27.337 | -27.337 | 0.000 |
| FeCl4-2 | 2.211e-031 | 1.010e-031 | -30.655 | -30.996 | -0.340 |
| Fe(OH)3- | 1.146e-031 | 9.453e-032 | -30.941 | -31.024 | -0.084 |
| Fe(OH)4-2 | 1.068e-039 | 4.881e-040 | -38.971 | -39.312 | -0.340 |
| Fe(3) | 2.385e-011 | | | | |
| Fe(OH)3 | 1.585e-011 | 1.585e-011 | -10.800 | -10.800 | 0.000 |
| Fe(OH)2+ | 7.959e-012 | 6.564e-012 | -11.099 | -11.183 | -0.084 |
| Fe(OH)4- | 2.493e-014 | 2.056e-014 | -13.603 | -13.687 | -0.084 |
| FeOH+2 | 8.228e-015 | 3.840e-015 | -14.085 | -14.416 | -0.331 |
| FeCO3+ | 1.639e-015 | 1.352e-015 | -14.785 | -14.869 | -0.084 |
| Fe+3 | 4.599e-019 | 1.152e-019 | -18.337 | -18.939 | -0.601 |
| FeSO4+ | 2.788e-020 | 2.299e-020 | -19.555 | -19.638 | -0.084 |
| FeNO3+2 | 1.563e-020 | 7.292e-021 | -19.806 | -20.137 | -0.331 |
| Fe(SO4)2- | 1.424e-021 | 1.175e-021 | -20.846 | -20.930 | -0.084 |
| FeCl2+ | 7.012e-022 | 5.783e-022 | -21.154 | -21.238 | -0.084 |
| FeCl+2 | 1.946e-022 | 9.078e-023 | -21.711 | -22.042 | -0.331 |
| Fe2(OH)2+4 | 7.251e-027 | 3.968e-028 | -26.140 | -27.401 | -1.262 |
| FeCl4- | 3.138e-029 | 2.588e-029 | -28.503 | -28.587 | -0.084 |
| FeNO2+2 | 3.095e-032 | 1.444e-032 | -31.509 | -31.840 | -0.331 |
| Fe3(OH)4+5 | 4.564e-035 | 5.442e-037 | -34.341 | -36.264 | -1.924 |
| H(0) | 0.000e+000 | | | | |
| H2 | 0.000e+000 | 0.000e+000 | -45.260 | -45.255 | 0.005 |
| K | 1.516e-005 | | | | |
| K+ | 1.486e-005 | 1.212e-005 | -4.828 | -4.917 | -0.089 |
| KSO4- | 2.898e-007 | 2.390e-007 | -6.538 | -6.622 | -0.084 |
| KCl | 2.243e-009 | 2.243e-009 | -8.649 | -8.649 | 0.000 |
| KOH | 2.170e-013 | 2.170e-013 | -12.664 | -12.664 | 0.000 |
| KHSO4 | 3.389e-014 | 3.389e-014 | -13.470 | -13.470 | 0.000 |
| Li | 4.998e-014 | | | | |
| Li+ | 4.924e-014 | 4.142e-014 | -13.308 | -13.383 | -0.075 |

| | | | | | |
|---|---|---|---|---|---|
| LiSO4- | 7.384e-016 | 6.090e-016 | -15.132 | -15.215 | -0.084 |
| LiCl | 7.999e-018 | 7.999e-018 | -17.097 | -17.097 | 0.000 |
| LiOH | 4.899e-021 | 4.899e-021 | -20.310 | -20.310 | 0.000 |
| Mg | 2.925e-003 | | | | |
| Mg+2 | 2.155e-003 | 1.135e-003 | -2.667 | -2.945 | -0.278 |
| MgSO4 | 6.636e-004 | 6.636e-004 | -3.178 | -3.178 | 0.000 |
| MgHCO3+ | 9.903e-005 | 8.168e-005 | -4.004 | -4.088 | -0.084 |
| MgCl+ | 6.583e-006 | 5.430e-006 | -5.182 | -5.265 | -0.084 |
| MgCO3 | 1.459e-006 | 1.459e-006 | -5.836 | -5.836 | 0.000 |
| Mg4(OH)4+4 | 3.835e-024 | 2.099e-025 | -23.416 | -24.678 | -1.262 |
| N(-03) | 0.000e+000 | | | | |
| N3- | 0.000e+000 | 0.000e+000 | -97.544 | -97.627 | -0.084 |
| HN3 | 0.000e+000 | 0.000e+000 | -99.593 | -99.593 | 0.000 |
| N(-3) | 0.000e+000 | | | | |
| NH4+ | 0.000e+000 | 0.000e+000 | -62.698 | -62.790 | -0.091 |
| NH3 | 0.000e+000 | 0.000e+000 | -65.471 | -65.471 | 0.000 |
| NH4SO4- | 0.000e+000 | 0.000e+000 | -73.763 | -73.847 | -0.084 |
| N(0) | 7.462e-018 | | | | |
| N2 | 3.731e-018 | 3.731e-018 | -17.428 | -17.428 | 0.000 |
| N(3) | 1.089e-016 | | | | |
| NO2- | 1.089e-016 | 8.876e-017 | -15.963 | -16.052 | -0.089 |
| HNO2 | 3.254e-020 | 3.254e-020 | -19.488 | -19.488 | 0.000 |
| FeNO2+2 | 3.095e-032 | 1.444e-032 | -31.509 | -31.840 | -0.331 |
| N(5) | 7.860e-003 | | | | |
| NO3- | 7.765e-003 | 6.331e-003 | -2.110 | -2.198 | -0.089 |
| CaNO3+ | 9.468e-005 | 7.809e-005 | -4.024 | -4.107 | -0.084 |
| HNO3 | 5.689e-011 | 5.689e-011 | -10.245 | -10.245 | 0.000 |
| FeNO3+2 | 1.563e-020 | 7.292e-021 | -19.806 | -20.137 | -0.331 |
| Na | 1.991e-002 | | | | |
| Na+ | 1.942e-002 | 1.601e-002 | -1.712 | -1.795 | -0.084 |
| NaSO4- | 3.203e-004 | 2.642e-004 | -3.494 | -3.578 | -0.084 |
| NaHCO3 | 1.582e-004 | 1.582e-004 | -3.801 | -3.801 | 0.000 |
| NaCl | 1.654e-005 | 1.654e-005 | -4.782 | -4.782 | 0.000 |
| NaCO3- | 1.011e-007 | 8.339e-008 | -6.995 | -7.079 | -0.084 |
| NaHSiO3 | 3.058e-008 | 3.058e-008 | -7.515 | -7.515 | 0.000 |
| NaAlO2 | 1.039e-009 | 1.039e-009 | -8.983 | -8.983 | 0.000 |
| NaOH | 9.471e-011 | 9.471e-011 | -10.024 | -10.024 | 0.000 |
| O(0) | 9.210e-004 | | | | |
| O2 | 4.605e-004 | 4.657e-004 | -3.337 | -3.332 | 0.005 |
| S(-2) | 0.000e+000 | | | | |
| H2S | 0.000e+000 | 0.000e+000 | -143.163 | -143.163 | 0.000 |
| HS- | 0.000e+000 | 0.000e+000 | -143.441 | -143.527 | -0.086 |
| S-2 | 0.000e+000 | 0.000e+000 | -149.565 | -149.888 | -0.322 |
| S2-2 | 0.000e+000 | 0.000e+000 | -254.473 | -254.813 | -0.340 |
| S3-2 | 0.000e+000 | 0.000e+000 | -359.438 | -359.778 | -0.340 |
| S4-2 | 0.000e+000 | 0.000e+000 | -464.633 | -464.973 | -0.340 |
| S5-2 | 0.000e+000 | 0.000e+000 | -570.049 | -570.389 | -0.340 |
| S(2) | 0.000e+000 | | | | |
| S2O3-2 | 0.000e+000 | 0.000e+000 | -147.660 | -148.000 | -0.340 |
| HS2O3- | 0.000e+000 | 0.000e+000 | -153.616 | -153.699 | -0.084 |
| S(3) | 0.000e+000 | | | | |
| S2O4-2 | 0.000e+000 | 0.000e+000 | -133.936 | -134.259 | -0.322 |
| S(4) | 0.000e+000 | | | | |
| HSO3- | 0.000e+000 | 0.000e+000 | -47.781 | -47.864 | -0.084 |
| SO3-2 | 0.000e+000 | 0.000e+000 | -48.024 | -48.355 | -0.331 |
| H2SO3 | 0.000e+000 | 0.000e+000 | -52.569 | -52.569 | 0.000 |
| SO2 | 0.000e+000 | 0.000e+000 | -52.746 | -52.746 | 0.000 |
| S2O6-2 | 0.000e+000 | 0.000e+000 | -69.060 | -69.400 | -0.340 |
| S3O6-2 | 0.000e+000 | 0.000e+000 | -176.531 | -176.871 | -0.340 |
| S4O6-2 | 0.000e+000 | 0.000e+000 | -267.919 | -268.259 | -0.340 |
| S5O6-2 | 0.000e+000 | 0.000e+000 | -388.494 | -388.834 | -0.340 |
| S(5) | 0.000e+000 | | | | |

```
  S2O5-2            0.000e+000  0.000e+000  -100.207  -100.548    -0.340
S(6)          7.309e-003
  SO4-2             5.466e-003  2.497e-003    -2.262    -2.603    -0.340
  CaSO4             8.586e-004  8.586e-004    -3.066    -3.066     0.000
  MgSO4             6.636e-004  6.636e-004    -3.178    -3.178     0.000
  NaSO4-            3.203e-004  2.642e-004    -3.494    -3.578    -0.084
  KSO4-             2.898e-007  2.390e-007    -6.538    -6.622    -0.084
  HSO4-             5.139e-008  4.239e-008    -7.289    -7.373    -0.084
  AlSO4+            4.233e-010  3.491e-010    -9.373    -9.457    -0.084
  Al(SO4)2-         8.205e-011  6.768e-011   -10.086   -10.170    -0.084
  KHSO4             3.389e-014  3.389e-014   -13.470   -13.470     0.000
  LiSO4-            7.384e-016  6.090e-016   -15.132   -15.215    -0.084
  H2SO4             8.909e-018  8.909e-018   -17.050   -17.050     0.000
  FeSO4+            2.788e-020  2.299e-020   -19.555   -19.638    -0.084
  FeSO4             2.718e-021  2.718e-021   -20.566   -20.566     0.000
  Fe(SO4)2-         1.424e-021  1.175e-021   -20.846   -20.930    -0.084
  NH4SO4-           0.000e+000  0.000e+000   -73.763   -73.847    -0.084
S(7)          0.000e+000
  S2O8-2            0.000e+000  0.000e+000   -42.995   -43.335    -0.340
S(8)          2.646e-029
  HSO5-             2.646e-029  2.183e-029   -28.577   -28.661    -0.084
Si            7.423e-005
  SiO2              7.415e-005  7.415e-005    -4.130    -4.130     0.000
  HSiO3-            4.464e-008  3.682e-008    -7.350    -7.434    -0.084
  NaHSiO3           3.058e-008  3.058e-008    -7.515    -7.515     0.000
  H2SiO4-2          4.744e-014  2.167e-014   -13.324   -13.664    -0.340
  H6(H2SiO4)4-2     4.016e-017  1.835e-017   -16.396   -16.736    -0.340
  H4(H2SiO4)4-4     5.713e-025  2.456e-026   -24.243   -25.610    -1.367
```

## A-15.2 Underlying Alluvium Sediments

The solution chemistry of the underlying alluvium sediment is not modeled. Instead, the effluent from the vault floor and sand/gravel base is assumed to be representative of the solution chemistry in the alluvium. These solution parameters are then used as a basis for recommending $K_d$ values from the literature.

## A-16. Model Validation

The model was validated by running a sample calculation from the PHREEQc users guide using the amended "llnl.dat" data file and then comparing these results with those published in the PHRREQc Users Manual (Parkhurst and Appelo, 1999, Water Resources Investigations Report 99-4359). The model calculation chosen was example #2, "Equilibration with Pure Phases." The input file for this example is

```
TITLE Example 2.--Temperature dependence of solubility
            of gypsum and anhydrite
SOLUTION 1 Pure water
      pH     7.0
      temp    25.0
EQUILIBRIUM_PHASES 1
      Gypsum        0.0     1.0
      Anhydrite     0.0     1.0
REACTION_TEMPERATURE 1
      25.0 75.0 in 51 steps
SELECTED_OUTPUT
      -file   ex2.sel
      -temperature
      -si     anhydrite  gypsum
END
```

The published results for this calculation are shown on the following two pages. The results from the validation calculation are shown after the published results. Comparison of the published results from the example problem with the result achieved when this example calculation was run match identically and validate the performance of the PHREEQc model for these studies. Any errors in calculation would be associated with incorrect parameter inputs or faulty assumptions and not computational errors associated with the operation of the PHREEQc code.

**Table 14.**--Selected output for example 2

```
------------------------------------------
Beginning of initial solution calculations.
------------------------------------------

Initial solution 1.     Pure water

-----------------------------Solution composition------------------------------

        Elements            Molality       Moles

        Pure water

----------------------------Description of solution----------------------------

                                     pH  =   7.000
                                     pe  =   4.000
                        Activity of water  =   1.000
                           Ionic strength  =   1.001e-07
                       Mass of water (kg)  =   1.000e+00
                Total alkalinity (eq/kg)   =   1.082e-10
                   Total carbon (mol/kg)   =   0.000e+00
                      Total CO2 (mol/kg)   =   0.000e+00
                     Temperature (deg C)   =  25.000
                  Electrical balance (eq)  =  -1.082e-10
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.05
                                Iterations  =   0
                                   Total H  = 1.110124e+02
                                   Total O  = 5.550622e+01

----------------------------Distribution of species----------------------------

                                                    Log       Log         Log
        Species             Molality    Activity  Molality  Activity     Gamma

        OH-                1.002e-07   1.001e-07    -6.999    -6.999    -0.000
        H+                 1.001e-07   1.000e-07    -7.000    -7.000    -0.000
        H2O                5.551e+01   1.000e+00     0.000     0.000     0.000
H(0)              1.416e-25
        H2                 7.079e-26   7.079e-26   -25.150   -25.150     0.000
O(0)              0.000e+00
        O2                 0.000e+00   0.000e+00   -42.080   -42.080     0.000

-----------------------------Saturation indices--------------------------------

        Phase               SI log IAP  log KT

        H2(g)           -22.00  -22.00    0.00  H2
        H2O(g)           -1.51    0.00    1.51  H2O
        O2(g)           -39.12   44.00   83.12  O2

------------------------------------------
Beginning of batch-reaction calculations.
------------------------------------------
```

```
Reaction step 1.

Using solution 1.       Pure water
Using pure phase assemblage 1.
Using temperature 1.

-------------------------------Phase assemblage-------------------------------

                                                    Moles in assemblage
        Phase               SI log IAP  log KT    Initial      Final      Delta

        Anhydrite         -0.22   -4.58   -4.36  1.000e+00             -1.000e+00
        Gypsum             0.00   -4.58   -4.58  1.000e+00  1.985e+00  9.849e-01

-----------------------------Solution composition-----------------------------

        Elements           Molality       Moles

        Ca                1.564e-02   1.508e-02
        S                 1.564e-02   1.508e-02

----------------------------Description of solution----------------------------

                                       pH  =   7.067      Charge balance
                                       pe  =  10.686      Adjusted to redox equilibrium
                          Activity of water  =   1.000
                             Ionic strength  =   4.178e-02
                          Mass of water (kg)  =   9.645e-01
                 Total alkalinity (eq/kg)  =   1.122e-10
                    Total carbon (mol/kg)  =   0.000e+00
                       Total CO2 (mol/kg)  =   0.000e+00
                     Temperature (deg C)  =  25.000
                   Electrical balance (eq)  =  -1.082e-10
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                                Iterations  =  19
                                   Total H  = 1.070728e+02
                                   Total O  = 5.359671e+01

----------------------------Distribution of species----------------------------

                                                    Log        Log        Log
        Species             Molality    Activity  Molality  Activity     Gamma

        OH-               1.417e-07   1.167e-07    -6.849    -6.933    -0.084
        H+                9.957e-08   8.575e-08    -7.002    -7.067    -0.065
        H2O               5.551e+01   9.996e-01    -0.000    -0.000     0.000
Ca                1.564e-02
        Ca+2              1.045e-02   5.176e-03    -1.981    -2.286    -0.305
        CaSO4             5.191e-03   5.242e-03    -2.285    -2.281     0.004
        CaOH+             1.204e-08   1.001e-08    -7.919    -7.999    -0.080
        CaHSO4+           3.166e-09   2.633e-09    -8.499    -8.580    -0.080
H(0)              4.383e-39
        H2                2.192e-39   2.213e-39   -38.659   -38.655     0.004
O(0)              1.685e-15
        O2                8.424e-16   8.505e-16   -15.074   -15.070     0.004
S(-2)             0.000e+00
        HS-               0.000e+00   0.000e+00  -117.646  -117.731    -0.084
        H2S               0.000e+00   0.000e+00  -117.860  -117.856     0.004
        S-2               0.000e+00   0.000e+00  -123.270  -123.582    -0.312
S(6)              1.564e-02
        SO4-2             1.045e-02   5.075e-03    -1.981    -2.295    -0.313
        CaSO4             5.191e-03   5.242e-03    -2.285    -2.281     0.004
        HSO4-             5.088e-08   4.231e-08    -7.293    -7.374    -0.080
        CaHSO4+           3.166e-09   2.633e-09    -8.499    -8.580    -0.080

-----------------------------Saturation indices-----------------------------

        Phase               SI log IAP  log KT

        Anhydrite         -0.22   -4.58   -4.36  CaSO4
        Gypsum             0.00   -4.58   -4.58  CaSO4:2H2O
        H2(g)            -35.51  -35.51    0.00  H2
        H2O(g)            -1.51   -0.00    1.51  H2O
        H2S(g)          -116.86 -158.45  -41.59  H2S
        O2(g)            -12.11   71.01   83.12  O2
        Sulfur           -87.23 -122.94  -35.71  S
```

# A-17. Results from Test Calculation

*REACTION STEP 1.*

```
Using solution 1.       Pure water
Using pure phase assemblage 1.
Using temperature 1.

-------------------------------Phase assemblage--------------------------------

                                                  Moles in assemblage
Phase               SI log IAP  log KT      Initial       Final       Delta

Anhydrite         -0.22   -4.58   -4.36   1.000e+000           0 -1.000e+000
Gypsum             0.00   -4.58   -4.58   1.000e+000  1.985e+000  9.849e-001

-------------------------------Solution composition--------------------------------

      Elements          Molality       Moles

      Ca              1.564e-002  1.508e-002
      S               1.564e-002  1.508e-002

----------------------------Description of solution----------------------------

                                pH  =  7.067     Charge balance
                                pe  =  10.685     Adjusted to redox equilibrium
     Specific Conductance (uS/cm, 25 oC) = 2160
                        Density (g/cm3)  =  0.99920
                     Activity of water  =  1.000
                       Ionic strength  =  4.178e-002
                    Mass of water (kg)  =  9.645e-001
               Total alkalinity (eq/kg)  =  1.122e-010
                 Total carbon (mol/kg)  =  0.000e+000
                   Total CO2 (mol/kg)  =  0.000e+000
                  Temperature (deg C)  =  25.000
                Electrical balance (eq)  = -1.082e-010
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =  -0.00
                           Iterations  =  17
                             Total H  = 1.070728e+002
                             Total O  = 5.359671e+001

----------------------------Distribution of species----------------------------

                                        Log      Log        Log
  Species             Molality    Activity  Molality  Activity     Gamma

  OH-               1.417e-007  1.167e-007    -6.849    -6.933    -0.084
  H+                9.957e-008  8.575e-008    -7.002    -7.067    -0.065
  H2O               5.551e+001  9.996e-001     1.744    -0.000     0.000
Ca            1.564e-002
  Ca+2              1.045e-002  5.176e-003    -1.981    -2.286    -0.305
  CaSO4             5.191e-003  5.242e-003    -2.285    -2.281     0.004
  CaOH+             1.204e-008  1.001e-008    -7.919    -7.999    -0.080
  CaHSO4+           3.166e-009  2.633e-009    -8.499    -8.580    -0.080
H(0)          4.397e-039
  H2                2.199e-039  2.220e-039   -38.658   -38.654     0.004
O(0)          1.674e-015
  O2                8.372e-016  8.453e-016   -15.077   -15.073     0.004
S(-2)         0.000e+000
  HS-               0.000e+000  0.000e+000  -117.641  -117.725    -0.084
```

```
  H2S                0.000e+000  0.000e+000  -117.855  -117.850     0.004
  S-2                0.000e+000  0.000e+000  -123.265  -123.577    -0.312
S(6)          1.564e-002
  SO4-2              1.045e-002  5.075e-003    -1.981    -2.295    -0.313
  CaSO4              5.191e-003  5.242e-003    -2.285    -2.281     0.004
  HSO4-              5.088e-008  4.231e-008    -7.293    -7.374    -0.080
  CaHSO4+            3.166e-009  2.633e-009    -8.499    -8.580    -0.080

-------------------------------Saturation indices--------------------------------

      Phase              SI log IAP  log KT

      Anhydrite       -0.22   -4.58   -4.36  CaSO4
      Gypsum           0.00   -4.58   -4.58  CaSO4:2H2O
      H2(g)          -35.50  -38.65   -3.15  H2
      H2O(g)          -1.51   -0.00    1.51  H2O
      H2S(g)        -116.85 -117.85   -1.00  H2S
      O2(g)          -12.18  -15.07   -2.89  O2
      Sulfur         -87.23  -82.35    4.88  S
```