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GEOCHEMICAL MODELING OF F AREA SEEPAGE BASIN COMPOSITION AND VARIABILITY

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Savannah River National Laboratory
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Prepared for the U.S. Department of Energy Under Contract Number DE-AC09-08SR22470

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REVIEWS AND APPROVALS

M. R. Millings, Environmental Restoration Technologies Date

B. B. Looney, Environmental Restoration Technologies Date

M. E. Denham, Environmental Restoration Technologies Date

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TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

1.0 EXECUTIVE SUMMARY

From the 1950s through 1989, the F Area Seepage Basins at the Savannah River Site (SRS) received low level radioactive wastes resulting from processing nuclear materials. Discharges of process wastes to the F Area Seepage Basins followed by subsequent mixing processes within the basins and eventual infiltration into the subsurface resulted in contamination of the underlying vadose zone and downgradient groundwater. For simulating contaminant behavior and subsurface transport, a quantitative understanding of the interrelated discharge-mixing-infiltration system along with the resulting chemistry of fluids entering the subsurface is needed. An example of this need emerged as the F Area Seepage Basins was selected as a key case study demonstration site for the Advanced Simulation Capability for Environmental Management (ASCEM) Program.

This modeling evaluation explored the importance of the wide variability in bulk wastewater chemistry as it propagated through the basins. The results are intended to generally improve and refine the conceptualization of infiltration of chemical wastes from seepage basins receiving variable waste streams and to specifically support the ASCEM case study model for the F Area Seepage Basins. Specific goals of this work included: 1) develop a technically-based "charge-balanced" nominal source term chemistry for water infiltrating into the subsurface during basin operations, 2) estimate the nature of short term and long term variability in infiltrating water to support scenario development for uncertainty quantification (i.e., UQ analysis), 3) identify key geochemical factors that control overall basin water chemistry and the projected variability/stability, and 4) link wastewater chemistry to the subsurface based on monitoring well data.

Results from this study provide data and understanding that can be used in further modeling efforts of the F Area groundwater plume. As identified in this study, key geochemical factors affecting basin chemistry and variability included: 1) the nature or chemistry of the waste streams, 2) the open system of the basins, and 3) duration of discharge of the waste stream types. Mixing models of the archetype waste streams indicated that the overall basin system would likely remain acidic much of the time. Only an extended periods of predominantly alkaline waste discharge (e.g., >70% alkaline waste) would dramatically alter the average pH of wastewater entering the basins.

Short term and long term variability were evaluated by performing multiple stepwise modeling runs to calculate the oscillation of bulk chemistry in the basins in response to short term variations in waste stream chemistry. Short term (½ month and 1 month) oscillations in the waste stream types only affected the chemistry in Basin 1; little variation was observed in Basin 2 and 3. As the largest basin, Basin 3 is considered the primary source to the groundwater. Modeling showed that the fluctuation in chemistry of the waste streams is not directly representative of the source term to the groundwater (i.e. Basin 3). The sequence of receiving basins and the large volume of water in Basin 3 "smooth" or nullify the short term variability in waste stream composition.

As part of this study, a technically-based “charge-balanced” nominal source term chemistry was developed for Basin 3 for a narrow range of pH (2.7 to 3.4). An example is also provided of how these data could be used to quantify uncertainty over the long term variations in waste stream chemistry and hence, Basin 3 chemistry.

2.0 PURPOSE

The F Area Seepage Basins at the Savannah River Site (SRS) received low level radioactive wastes resulting from processing nuclear materials. The basins operated from the 1950s through 1989 and then were stabilized, closed and capped. During operation, discharges of process wastes to the F Area Seepage Basins, subsequent mixing processes within the basins and eventual infiltration into the subsurface resulted in contamination of the underlying vadose zone and downgradient groundwater. Developing a quantitative understanding of the interrelated discharge-mixing-infiltration processes and the resulting chemistry of fluids entering the subsurface is important for simulating contaminant behavior and subsurface transport. Significant and diverse data on waste characteristics, groundwater, surface water and vadose zone contaminant concentrations, basin construction and operation, and related topics are available for the F Area Seepage Basins.

Based on the subsurface simulation needs/challenges and the available supporting data, the field research site associated with the F Area Seepage Basins was selected as a key case study demonstration site for the Advanced Simulation Capability for Environmental Management (ASCEM) Program. In gathering data for this specific initiative, the geochemical compositions of the waste streams and seepage basins emerged as important topics. Although the total waste stream volume and discharged activity of most key radionuclides (except I-129) are relatively well documented (Cummins et al., 1991), several challenges remain. For example, to support coupled geochemical modeling, the available data on the quantity of contaminants and total volume of wastewater must be supplemented with information on the nature and variability in the bulk chemistry. The required supplemental information includes parameters such as ionic strength, major cations and anions, and master variables such as pH. Furthermore, mixing within the basins prior to infiltration would modify the bulk source term entering the subsurface and would influence the mobility of contaminants in the near-field vadose and groundwater environment.

The general purpose of this evaluation is to explore the importance of the wide variability in bulk wastewater chemistry as it propagates through the basins and to estimate the resulting dampened variability in seepage basin water chemistry (the source term to the subsurface). The results are intended to generally improve and refine the conceptualization of infiltration of chemical wastes from seepage basins receiving variable waste streams and to specifically support the ASCEM case study model for the F Area Seepage Basins. Specific goals of this work include: 1) develop a technically-based “charge-balanced” nominal source term chemistry for water infiltrating into the subsurface during basin operations, 2) estimate the nature of short term and long term variability in infiltrating water to support scenario development for uncertainty quantification (i.e., UQ analysis), 3) identify key geochemical factors that control overall basin water chemistry and the projected variability/stability, and 4) link wastewater chemistry to the subsurface based on monitoring well data. This report describes the inputs and assumptions used in the simulations in addition to documenting and discussing the results.

3.0 MODELING APPROACH

We simulated varying waste stream composition using historical data, The Geochemist's Workbench (Release 8.0, Bethke and Yeakel 2009) (GWB), and a simplified basin mixing scenario. Primary sources of information related to bulk waste stream composition include Ryan (1984) and related summaries (e.g., Killian, 1985), as well as historical and periodic reports of total quantities of nitrate or caustic discharged. The various references document that, in general, the wastewater chemistry was either strongly acidic or strongly basic depending on the processing campaign in operation at any particular time. The widely varying chemistry limits the accuracy of simple averaging to generate a charged-balanced nominal waste mixture. Instead, we developed a scenario based approach using periodic discharges of archetype acidic and basic wastewater to estimate the magnitude of pH (and bulk chemistry) oscillation in Basins 1, 2 and 3 assuming known basin volumes and complete mixing in each basin. The Ryan data were collected over a relatively short period of time (4^{th} quarter, 1983) and appropriate strategies for application of the available information to 35 years of operation were developed according to historical near-field groundwater chemistry data.

The evaluation was performed in a stepwise-sequential manner as shown in Figure 1. As shown, we used the following steps to simulate the propagation of varying waste steam composition through the F Area Seepage Basin cascade:

- Developed inputs and assumptions according to available historical data
- Generated archetype waste stream chemistries using GWB
- Created a simplified model of basin mixing and flow assuming a Completely Stirred Tank Reactor (CSTR),
- Used GWB to calculate charge balanced basin chemistries, and
- Documented basin chemistries for a range of scenarios related to the duration of waste stream variation.
- Generated a more detailed charge balanced source term chemistry as a function of pH
- Assessed historical groundwater data from near-field centerline wells to generate statistics to support UQ analysis.

The details and assumptions associated with each step – for example how GWB was used to simulate basin mixing in a CSTR– are described in more detail in the following sections.

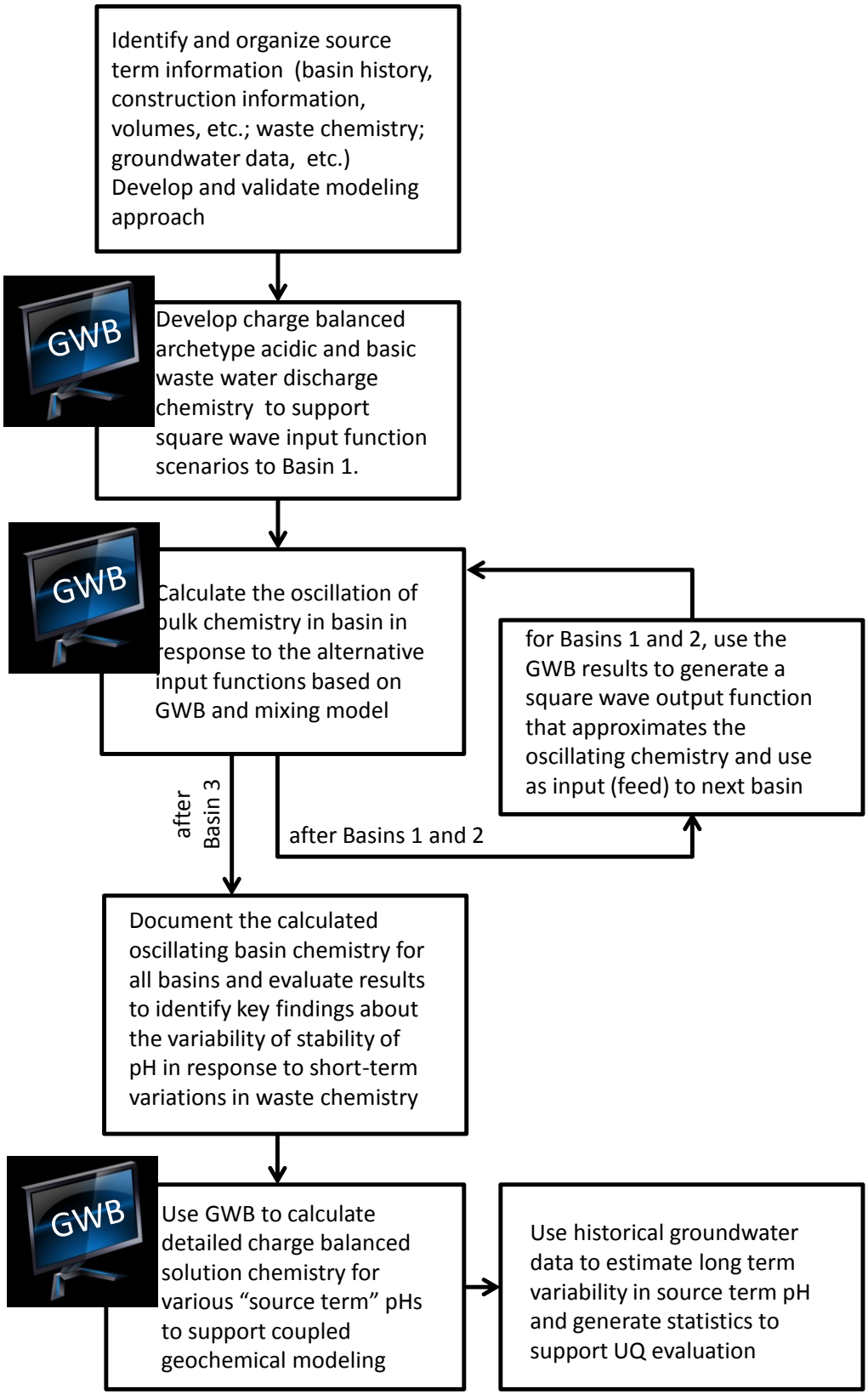


Figure 1. Stepwise approach used in modeling the F Area Seepage Basins Chemistry

3.1 GENERAL INPUTS AND ASSUMPTIONS

Table 1 provides some of the key inputs and assumptions used in this analysis.

Table 1. Input and Assumptions

Inputs/Assumptions		Reference
• Approximate Basin Volumes		
Basin 1 =	*3.9 million liters*	Killian (1985)
Basin 2 =	*7.4 million liters*	
Basin 3 =	*53 million liters*	
• Approximate Monthly Waste Stream Volume		
To Basin 1 =	*13 million liters*	Killian (1985) (estimate based on average daily flow of 411 m^3/day in 1985)
• Duration of high pH waste stream estimated between 15 and 30 days		Ryan (1984)
• Lowest pH observed in nearby groundwater wells		
pH 2.7 =	*FSB78*	Killian (1985)
Other wells with pH < 3.0	*FSB79, FSB94D&DR, FSB95D&DR, FSB110D*	ERDMS database (collection dates range from 1985-2005)
• Waste stream enters Basin 1 via an underground pipeline. Basin 1 flows via an underground pipeline to Basin 2. Basin 2 flows via an underground pipeline to Basin 3.		Killian (1985)
• Basins 1 and 2 had relatively low seepage rates		Oral history

3.2 GENERIC WASTE STREAM CHEMISTRY

Generic or baseline waste stream chemistries were derived according to available historical information (Appendix C.1 in Ryan 1984). As part of a 1983 sampling program of the waste streams from the separations area, the F-Area trebler (source to the seepage basins) was sampled twice a month for approximately four months. Major cations, anions and field parameters were included with the radionuclides that were analyzed. As shown by these data, the waste stream varied between an acidic nitrate waste stream (pH~2.5, 1000 to 6000 mg/L nitrate) and an alkaline waste stream (pH~12).

Analytical data from the sampling program were used as input to GWB to generate charge balanced archetype acidic and alkaline waste streams. A simplistic bulk chemical composition was used for both waste streams to include major cations and anions with only a few minor ions. Both waste streams were charge balanced using nitrate. The alkaline waste stream was saturated with respect to some minerals; however these were not allowed to precipitate prior to mixing with basin water. Table 2 provides the chemical compositions for the archetype waste streams used in GWB.

Table 2. Chemistry of Generic Waste Streams

Waste Stream Chemistry	Moles per L	Converted Concentration	
Generic Acidic Waste Stream			
H+	3.24E-03	2.49	pH
NO3-	3.57E-02	2214	mg/L
Na+	3.24E-02	745	mg/L
SiO2(aq)	3.29E-05	2	mg/L
Generic Alkaline Waste Stream			
H+	8.84E-13	12.05	pH
NO3-	1.43E-03	89	mg/L
Na+	1.65E-02	378	mg/L
SiO2(aq)	9.04E-05	5	mg/L
Ca+2	1.06E-04	4	mg/L
Carbonate Alkalinity as CaCO3	6.05E-04	61	mg/L

3.3 MODELING BASIN CHEMISTRY AND MIXING

We used the flash mixing option of GWB to simulate a CSTR in order to mix the generic waste streams and basin waters. The following sections explain the relationship between GWB's flash mixing option and a CSTR. We also describe the workflow for the modeling runs performed to evaluate each basin's chemistry. Lastly, we provide information regarding the two waste stream scenarios modeled to evaluate variability in the duration of waste stream discharge.

3.3.1 Calculating Hypothetical Basin Chemistries

3.3.1.1 Relating the CSTR to Flash Mixing in GWB

The assumption that the seepage basins can be approximated as a cascade of CSTRs is central to developing a practical approach for applying geochemical models to relate time varying effluent chemistry to the time varying solution composition in Basin 3. A key feature of geochemical models, such as GWB, is the ability to mix two solutions and generate the solution chemistry of the resultant mixture. This "flash mixing" is performed as depicted in Figure 2a. In this case, some fraction of the original solution (solution A) is removed and replaced with an equal volume of solution B. The flash mix ratio (β_f) is simply defined as the fraction of solution A that was replaced. As shown, β_f ranges from 0 (i.e., 100% solution A) to 1 (i.e., 100% solution B). The mixing in a CSTR (Figure 2b) is distinctly different than flash mixing. In this case, a step change to solution B results in mixing, but some of the solution B is lost in the effluent and the fraction of the Basin that is solution B builds up slowly over time. The ratio of the volume of solution B inflow to the initial volume of basin fluid is the "normalized cumulative basin turnover" (τ_V) and is calculated as shown in Figure 2b. While τ_V for a CSTR is analogous to the β_f for flash mixing, the values for τ_V can range from 0 (i.e., basin contains 100% solution A) to infinity (solution contains 100% Solution B); in practical terms, values of τ_V greater than about 4 would contain over 98% solution B.

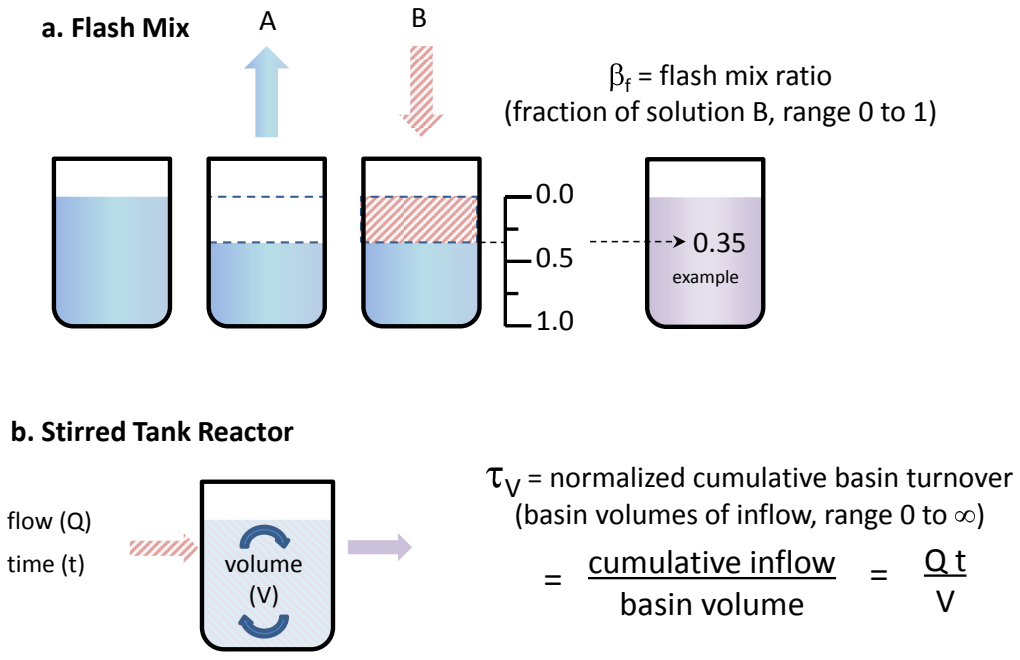


Figure 2. Comparison of Flash Mixing and a CSTR

The quantitative behavior of flash mixing versus mixing in a CSTR for a conservative constituent introduced as a step function is shown in Figure 3. As described above, the concentration of a flash mixing ranges in direct proportion to β_f while the CSTR moves from solution A to Solution B exponentially. Importantly, for solutions where the mixing is well behaved and where formation/loss of solid phases is minimal, there is an explicit theoretical relationship between the solution compositions for flash mixing and a CSTR; the value of τ_V for any CSTR can be mapped to an equivalent β_f for flash mixing using the following equation:

$$\beta_f = 1 - e^{-\tau_V} \qquad \text{(Equation 1)}$$

Thus, to a reasonable approximation, the real-world physical parameters associated with a CSTR basin receiving process wastes (e.g., flow, volume and time) can be related to the flash mixing paradigm in standard geochemical models to assess the impacts of oscillating (or changing) waste concentrations.

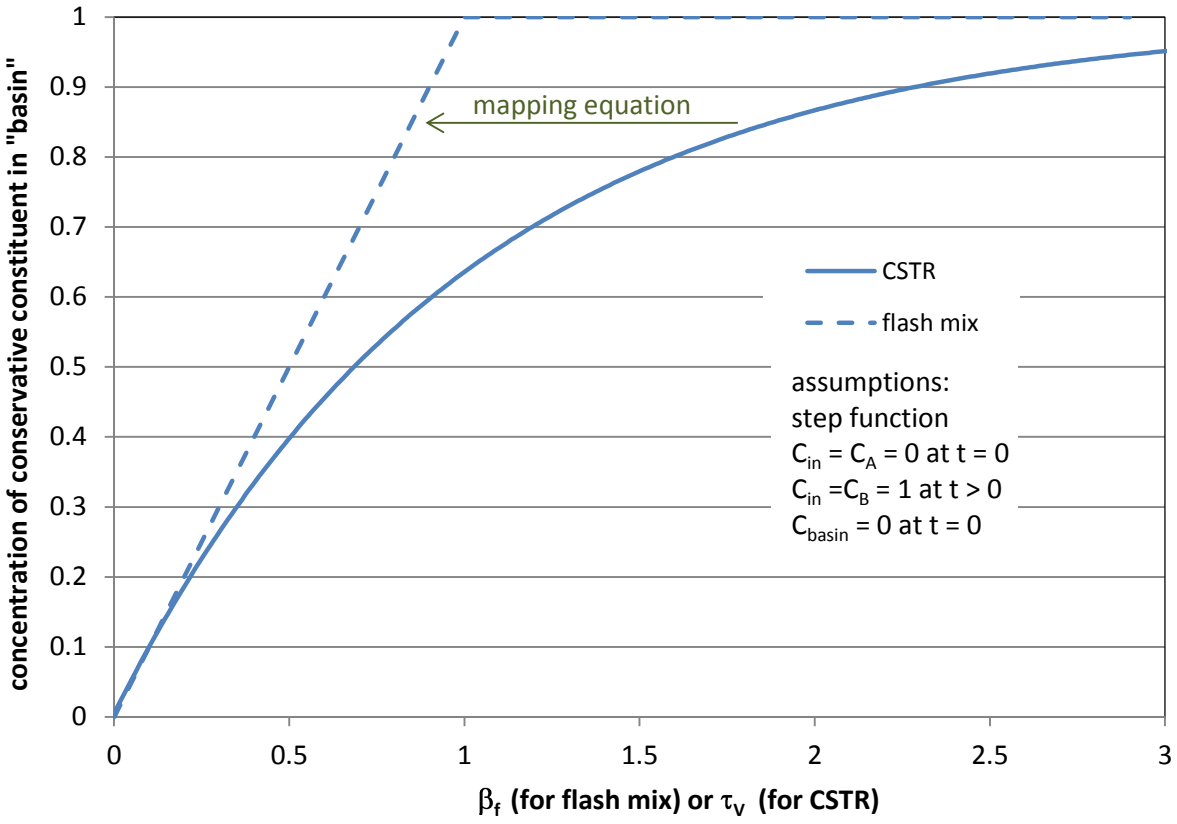


Figure 3. Comparison of flash mixing and CSTR mixing behaviors

3.3.1.2 Modeling Workflow

We used the "flash" mixing option in GWB along with Equation 1 to approximate the chemistry of each basin and the input chemistry for each subsequent basin (Figure 4). For all of these modeling runs, nitrate was used to charge balance, sorption and mineral precipitation were ignored, and the system was open to the atmosphere (log fO_2 = -0.699 and log fCO_2 = -3.5). The workflow for the modeling runs consisted of a cascade of CSTRs. The specific modeling steps (or runs) are outlined below.

1) Initially, an acidic waste stream (pH ~2.5) was assumed to discharge to Basin 1 for a specified period of time where it mixed with Basin 1 water. The output file (chemistry) from this mixing was used as the Basin 1 composition for the next step.
2) An alkaline waste stream was then assumed to discharge to Basin 1 for a specified period of time where it mixed with Basin 1 water. The output file (chemistry) from this mixing was used as the Basin 1 composition for the next step.
3) Steps 1 and 2 were repeated multiple times to calculate a generic acidic Basin 1 chemistry and a generic alkaline Basin 1 chemistry. These generic acidic and alkaline Basin 1 chemistries were used as inputs in the next three steps.
4) The acidic Basin 1 chemistry was assumed to discharge to Basin 2 for a specified period of time where it mixed with Basin 2 water. The output file (chemistry) from this mixing was used as the Basin 2 composition for the next step.
5) The alkaline Basin 1 chemistry was assumed to discharge to Basin 2 for a specified period of time where it mixed with Basin 2 water. The output file (chemistry) from this mixing was used as the Basin 2 composition for the next step.
6) Steps 4 and 5 were repeated multiple times to calculate a generic acidic Basin 2 chemistry and a generic alkaline Basin 2 chemistry. These generic acidic and alkaline Basin 2 chemistries were used as inputs in the next three steps.
7) The acidic Basin 2 chemistry was assumed to discharge to Basin 3 for a specified period of time where it mixed with Basin 3 water. The output file (chemistry) from this mixing was used as the Basin 3 composition for the next step.
8) The alkaline Basin 2 chemistry was assumed to discharge to Basin 3 for a specified period of time where it mixed with Basin 3 water. The output file (chemistry) from this mixing was used as the Basin 3 composition for the next step.
9) Steps 7 and 8 were repeated multiple times to calculate an overall Basin 3 chemistry, which would serve as a potential source of groundwater contamination.

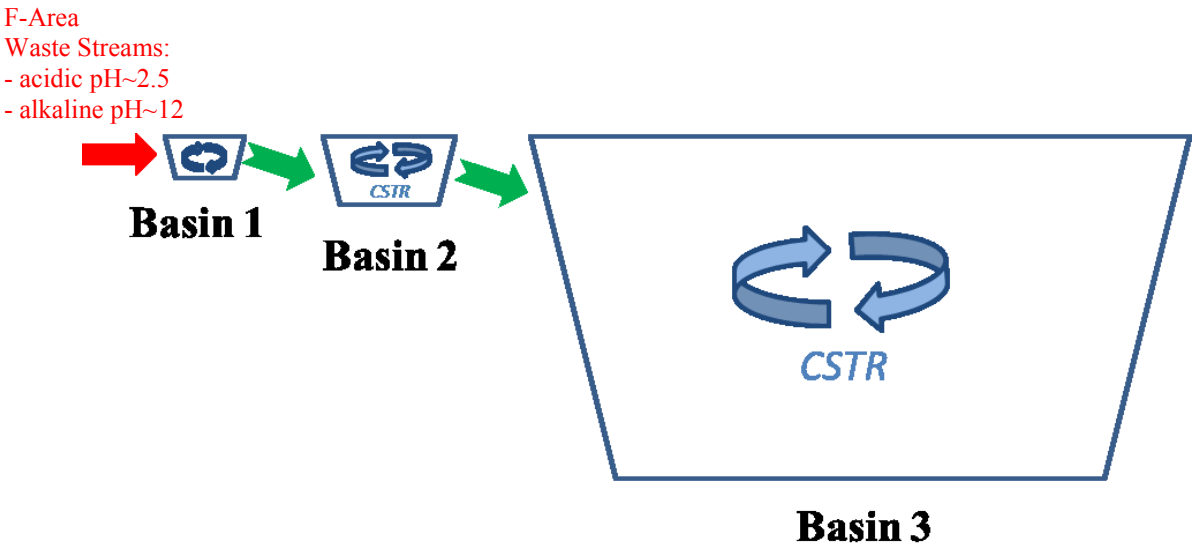


Figure 4. General Workflow for Calculating Basin Chemistry

3.3.1.3 Conceptual Model

Figure 5 depicts our conceptual model for pH of the discharge streams and basins. We expected that the large swings in pH of the discharge stream would be smoothed by the mixing of water in the receiving basin. In Figure 5, the vertical axis represents pH and the horizontal axis reflects time. The blue line represents pH of the discharge stream; it fluctuates between an acidic stream and an alkaline stream. The dashed, black oscillating line represents pH of the basin water and would be calculated assuming a CSTR (using the flash mix in GWB and Equation 1).

For ease in our calculations, we used a simplified square wave (stair step) function to approximate the basin water's composition (as represented by the dashed, red stair step line). The approximated acidic and alkaline chemistries (the top and bottom of the dashed red line) were then used as acidic and alkaline inputs (discharge streams) into the next basin.

Note that the CSTR assumption and the square wave input function are simplifications that would not precisely match the real-world conditions. In a real basin, the mixing would not be instantaneous and complete (for example, a real basin may form a thermocline or a chemocline during some periods with less mixing in the bottom waters and the potential for periodic depletion of dissolved oxygen). Nonetheless, the simplification provides a tractable method to approximate the most important features of the oscillating chemistry and to link a robust geochemical model to a complex surface water system. Available field data (e.g., all near-field groundwater has significant levels of dissolved oxygen) generally support the conceptual model and assumptions used in the modeling.

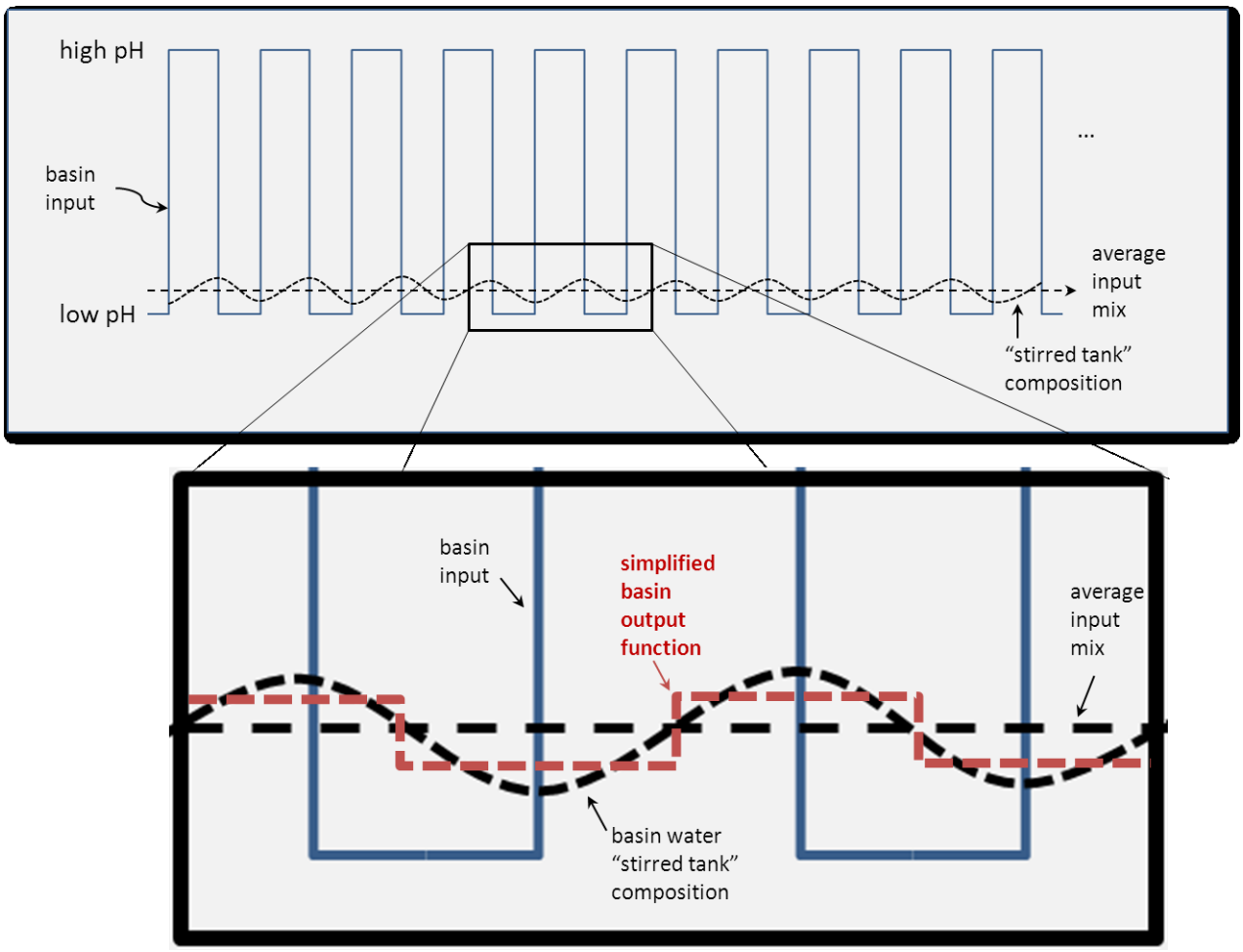


Figure 5. Conceptual Model of pH in Discharge Streams and Basins

3.3.2 Evaluating Effects of Disposal Duration

We modeled two different waste stream scenarios to assess the effects of disposal duration on basin chemistries. One scenario assumed ½ month alternating disposal cycles (½ month of acidic waste with a pH ~2.5 and ½ month of alkaline waste with a pH ~12) and the other scenario assumed 1 month alternating disposal cycles (1 month of acidic waste with a pH ~2.5 and 1 month of alkaline waste with a pH ~12). Figure 6 depicts the two scenarios with the green line representing the ½ month cycle and the blue dashed line representing the 1 month cycle. Modeling for each scenario began halfway through the acidic cycle and then ran for a minimum of three full cycles (e.g., an alkaline cycle, an acidic cycle and an alkaline cycle).

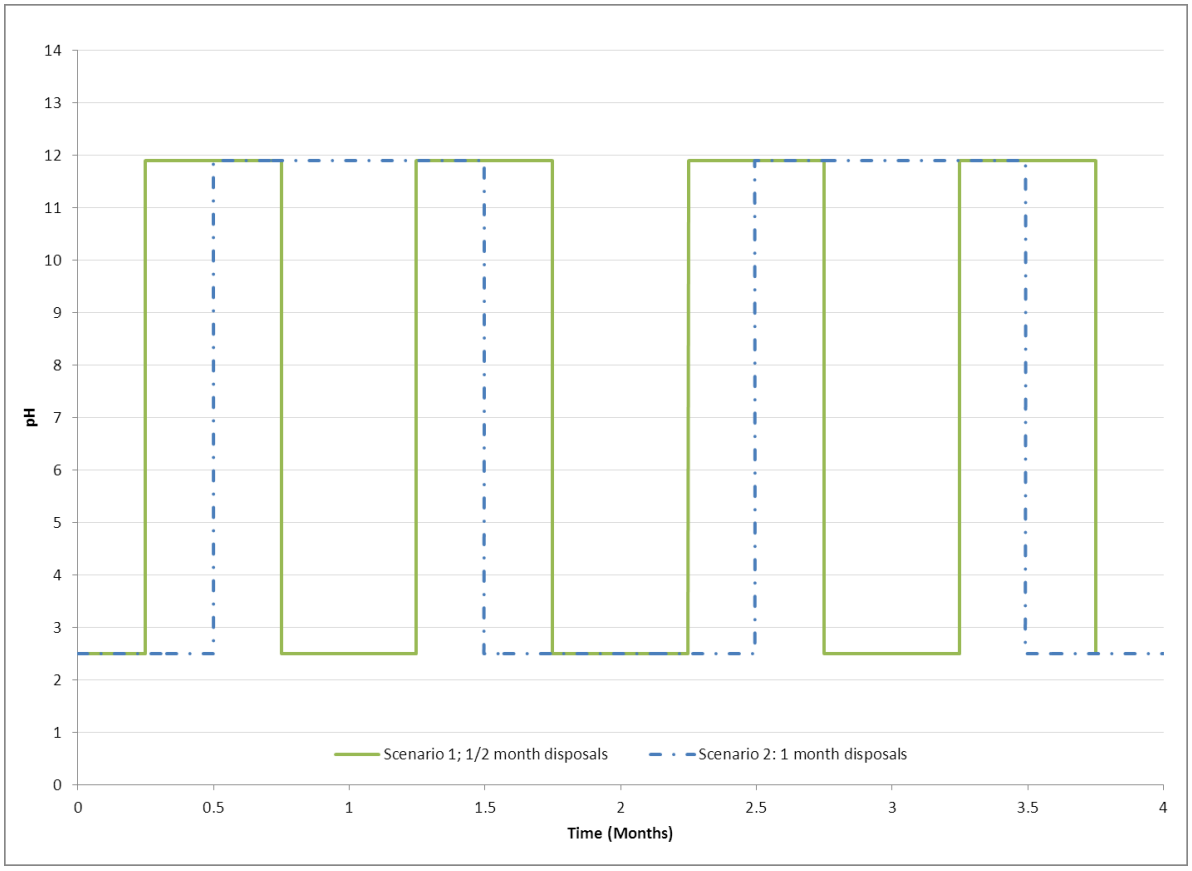


Figure 6. Duration of Waste Stream Discharge Scenarios

3.4 MODELING RESULTS AND DISCUSSION

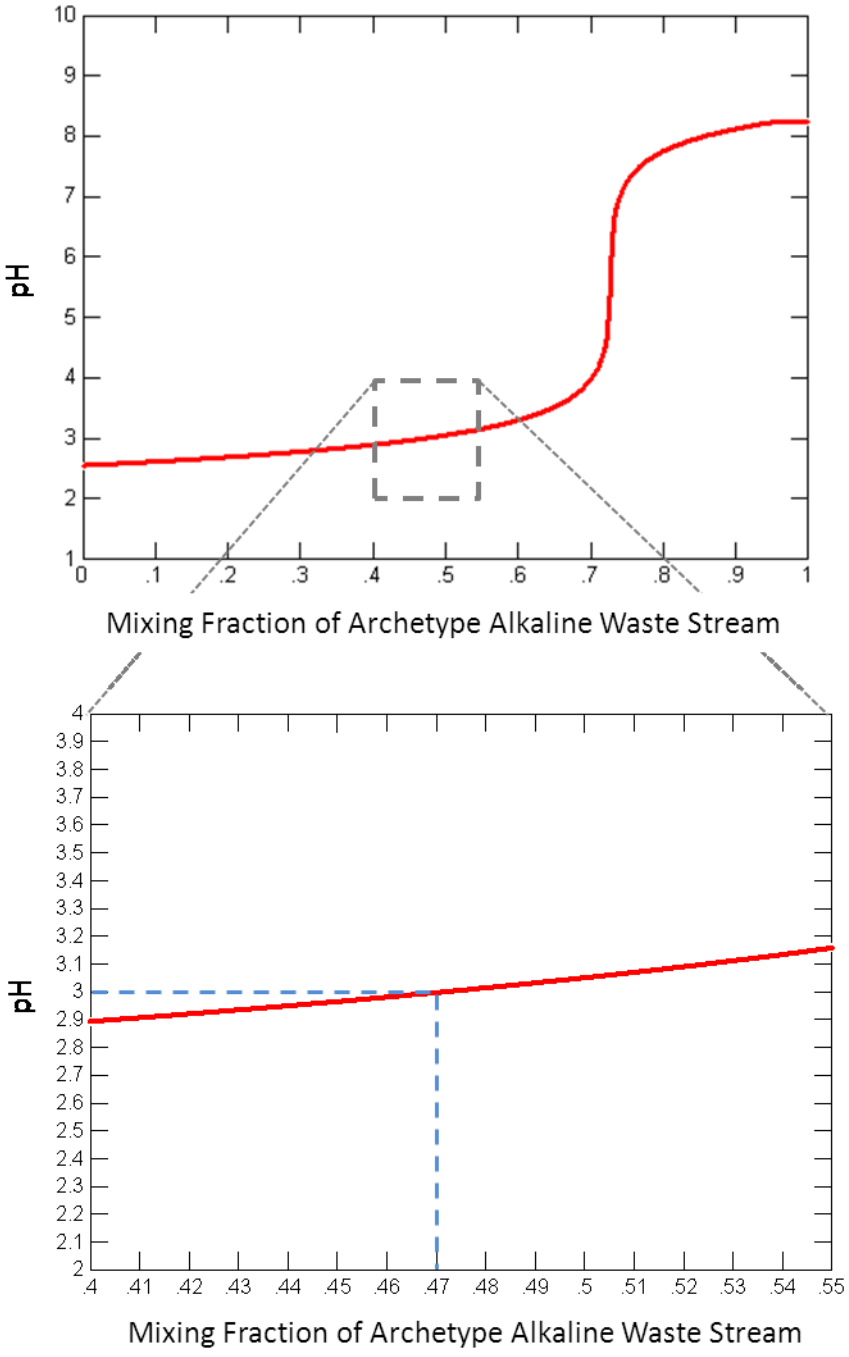
3.4.1 Archetype Waste Streams

Facility processes in F Area produced highly acidic and highly alkaline waste streams that were discharged to the seepage basins. However, there is limited knowledge regarding the specifics of duration and chemical composition of the waste streams. Sampling performed in the early 1980's indicated a cyclic discharge scenario where an acidic waste stream was discharged for 15 to 30 days followed by the discharge of an alkaline waste stream for 15 to 30 days. Although this sampling only reflects facility processes during the period of sampling, it gave us a starting place for modeling of the waste streams. We also know from groundwater monitoring data that the groundwater plume emanating from the seepage basins was primarily acidic suggesting that the source term (primarily Basin 3) was acidic.

Mixing of the archetype waste streams was modeled to gain further insight as to the fraction of each waste stream type that would be discharged to produce hypothetical basin water with a pH ~3.0. Figure 7 shows the pH that results from mixing a fraction of the alkaline waste stream with a fraction of the acidic waste stream (e.g., Figure 2a). For this modeling, we incorporated the flash mix option in GWB, assumed an open system (log fO2 = -0.699 and log fCO2 = -3.5), ignored sorption, but allowed mineral precipitation. At a pH >8.32, calcite becomes oversaturated and precipitates. However, it should be noted that the archetype waste types assumed simplistic chemistries consisting only of primary chemical constituents. With the addition of minor elements, other mineral precipitation might also be favored.

As shown by the mixing reaction (Figure 7), a solution with a pH ~3.0 occurs by mixing roughly half of the alkaline waste stream with half of the acidic waste stream (to be exact, 53% of the acidic waste stream and 47% of the alkaline waste stream). Also noteworthy is the fact that in mixing the two waste streams, the pH primarily remains acidic up to a mixing fraction of about 30% of the acidic waste stream and 70% of the alkaline waste stream. At this point (~70% alkaline waste stream), the pH steadily rises, but does not exceed a pH ~8.3 because of the fixed open system. The acidic nature of the solution results from two things – 1) the logarithmic scale of pH leads to a system still overwhelming dominated by H+ ions even with the addition of a strong base and 2) the open atmosphere, which provides a constant source of CO2(gas), enables the formation of HCO3-, which buffers the system and prevents a high pH.

Mixing of the two archetype solutions provides some understanding as to the likely chemistry of the basins. For example, we would expect that in Basin 1, the basin which directly receives the waste streams from F Area, the pH might swing from about 2.5 to 8.2 with the oscillations in waste streams depending on discharge duration (no higher or lower). We would also expect that the overall system would be acidic much of the time unless there was an exceeding long period (perhaps a year or more) during the process campaign when only alkaline waste was discharged.



Note: values on the x axis are the fraction of archetype alkaline waste with the remainder of the mixture consisting of archetype acid waste (e.g., 0.45 alkaline waste → 0.55 acid waste)

Figure 7. Mixing of Archetype Waste Streams

3.4.2 Short term Variability

We performed multiple stepwise modeling runs to calculate the oscillation of bulk chemistry in the basins in response to short term variations in waste stream chemistry. For purposes of our evaluation, "short term variability" represents changes in composition in the ½ month to 1 month timeframe. For example, the oscillations from an acidic waste stream to an alkaline waste stream that we modeled are considered short term. "Long term variability" denotes changes in composition in the 6 month to year (or longer) timeframe. Long term variability would reflect process changes and campaigns by the F Area facility.

Appendix A provides a summary table for the modeling runs performed to evaluate effects from the oscillating waste stream. The table includes the following information:

- The fraction of monthly flow each basin received (assuming an approximate flow rate of 13 million liters per month) per disposal cycle
- The volume of water each basin received per disposal cycle
- Type of influent each basin received per disposal cycle (acidic or alkaline)
- The equivalent flash mix ratio (see Figure 3) per disposal cycle
- The approximate pH of the influent water (for Basin 1, the pH represents the archetype waste streams; for Basins 2, pH represents output from Basin 1; for Basin 3, pH represents output from Basin 2)
- The output pH, which reflects mixing of the basin water with the influent water.

GWB output files for the ½ month waste stream discharge and 1 month waste stream discharge are provided in Appendix B and Appendix C. These output files only include the specified flash mix ratio used in the modeling runs (see Appendix A for flash mix ratio). Modeling runs were setup so that the flash mix ratio value was equivalent to the modeling time step (e.g., flash mix ratio of 0.565 = the time step #565).

Table 3 provides a summary of observed changes in pH for each basin. Figure 8 graphically shows pH changes in each basin for the ½ month discharge duration and 1 month discharge duration. To easily assess the effect of discharge duration, the graphs are provided side by the side for each basin. For each graph, the y axis reflects pH and the x axis reflect time in months (0 to 2 months for graphs on the left and 0 to 5 months for graphs on the right). Note that for Basin 1, the vertical axis shows pH from 2 to 12 in 1 pH unit intervals; for Basin 2, the vertical axis shows pH from 2.5 to 3.7 in 0.2 pH unit intervals; and for Basin 3, the vertical axis shows pH from 2.7 to 3.3 in 0.1 pH unit intervals. The top graphs (Basin 1) also provide pH of the influent waste water (green dashed line).

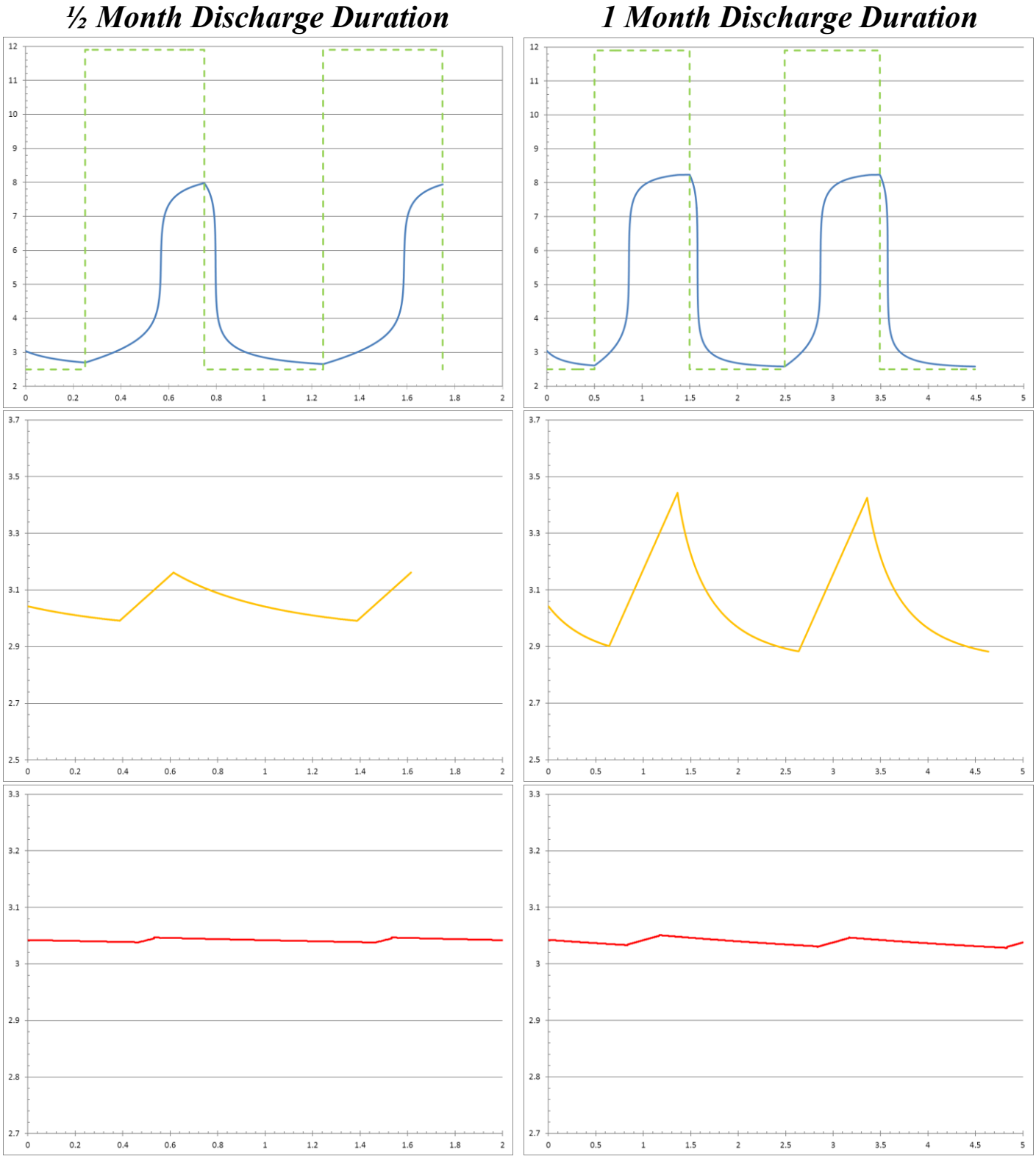
Table 3. Observed Changes in Model pH of Basin Water

Basin	Estimated Volume (million liters)	Changes in pH of Basin Water Chemistry	
		1/2 month scenario	1 month scenario
Basin 1	3.9	sharp changes in pH	sharp changes in pH; basin water approaches the pH of actual waste stream
Basin 2	7.4	little change in pH (a few decimal pH units)	moderate change in pH (~1/2 pH unit)
Basin 3	53	Little change in overall pH	Little change in overall pH

For Basin 1, changes in influent waste stream chemistry directly impact the pH of the basin water (Figure 8). For the ½ month discharge scenario, pH varies between 2.7 and 8.0. For the 1 month discharge scenario, the basin water becomes slightly more acidic (pH 2.6) and more alkaline (pH 8.2) during the discharge events. During the longer, 1 month discharge duration, the period of alkaline conditions in the basin is much longer than the ½ month scenario. Under these conditions, the basin water would likely be episodically saturated with respect to certain minerals (e.g., calcite, aragonite). The calculated swings in pH would also influence natural minerals present in the underlying basin sediments, resulting in colloid generation, shrinking and swelling of clays, and other physical changes that would tend to clog or occlude flow. Thus, pH conditions such as the ones modeled suggest that mineral precipitation either in the waste stream or in the basin combined with interactions of the solution with underlying sediments could have contributed to plugging of the basin and the modeling results are consistent with the oral history for the site.

Modest levels of mineral precipitation and dissolution were projected to occur in Basin 1 in response to projected pH oscillations. While this involved a relatively small portion of the elemental mass, such precipitation would contribute to infiltration reduction due to plugging of the underlying sediments. In addition, mineral precipitation would damp/buffer the uppermost extremes of the basin pH cycles. For example, at times of extended discharge of highly alkaline wastes, precipitation of calcite and/or dissolution of kaolinite would buffer basin pH keeping the basin water from reaching the highest calculated pH values. Similarly, at times of highly acidic discharges, the dissolution of calcite and kaolinite would buffer basin pH. Minerals that precipitated in the waste stream or in Basin 1 during alkaline discharges would have settled into basin sediments, remained in solution, or been transported to Basin 2 where they would redissolve in the consistently acidic conditions described below.

Basin 2 receives influent water from Basin 1 and is approximately twice the size of Basin 1. Our modeling results suggest that the Basin 2 chemistry is less impacted by the oscillating acidic and alkaline F-Area waste streams. For the ½ month discharge scenario, pH varies between ~3.0 and ~3.2. For the 1 month discharge scenario, the basin water becomes slightly more acidic (pH ~2.9) and slightly more alkaline (pH ~3.4) during the discharge events.



Notes: Basin 1 vertical axis shows pH from 2 to 12 in 1 pH unit intervals; Basin 2 vertical axis shows pH from 2.5 to 3.7 in 0.2 pH unit intervals; Basin 3 vertical axis shows pH from 2.7 to 3.3 in 0.1 pH unit intervals. Horizontal axis reflects time (left = 0 to 2 months; right = 0 to 5 months)

Figure 8. pH vs Time in Each Basin for ½ Month Discharge and 1 Month Discharge

Both discharge scenarios show that the pH of Basin 3 is practically unaffected by the fluctuations in F-Area waste stream chemistry (i.e., the influent to Basin 1). As the largest of the basins, Basin 3 would have contributed the greatest volume of contaminated water to the groundwater. Even though Basin 1 did show a fluctuating pH, its small size and oral history of showing little seepage would have little impact to the groundwater compared to Basin 3. Hence, the fluctuation in chemical composition of the F-Area waste stream discharged to the basins is not directly representative of the source term to the groundwater. The sequence of receiving basins and the large volume of water in Basin 3 would have "smoothed" or nullified the short term variability in waste stream composition.

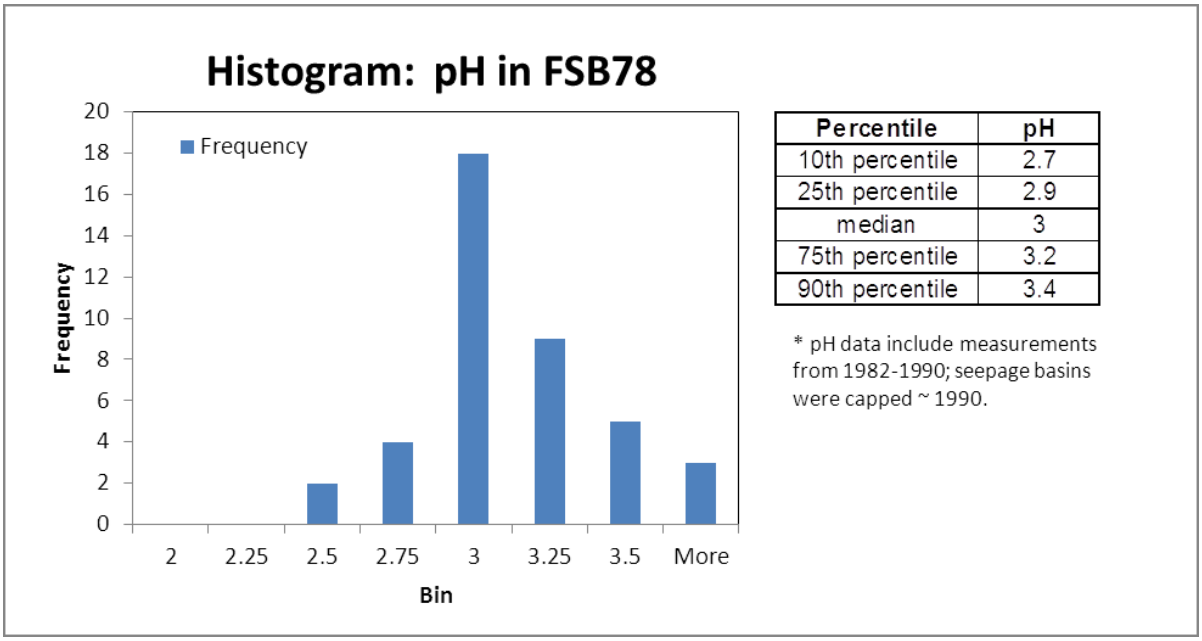
3.4.3 Source Term Chemistry and Groundwater Data

Since Basin 3 was the greatest source to the groundwater, pH data for the groundwater can serve as a constraint on the chemistry of Basin 3. When we started our modeling, we made an assumption that Basin 3 water had a pH ~3. Upon further review of historical groundwater data and reports, we know that pH values lower than 3 have been measured in the groundwater (Appendix D). Consequently, it is likely that Basin 3 chemistry at some point had a pH lower than 3.

To support further ASCEM modeling efforts, we modeled a more detailed charge balanced solution chemistry for Basin 3, the source term for the F Area groundwater plume. Since the water in Basin 3 likely had a pH less than 3.0 for some duration of time, we provide a charge balanced chemistry for various pH's to include 2.7, 2.9, 3.0, 3.2, and 3.4. We derived this range in chemistry according to the data we reviewed for FSB78 data (Figure 9 and Appendix D). FSB78 is located along the main flowpath downgradient of Basin 3 (i.e., the core of the groundwater plume) and therefore is a good representation of water emanating from Basin 3.

Groundwater measurements of pH are available for FSB78 starting in 1982. For our evaluation, we included groundwater measurements through 1990, which corresponds to the approximate time when the seepage basins were capped. Figure 9 provides a histogram and statistics for pH in FSB78. These statistics can be used to estimate long term variability in Basin 3 chemistry (the source term) and to generate statistics to quantifying uncertainty.

Appendix E includes a charge balanced chemistry for Basin 3 at pH 2.7, 2.9, 3.0, 3.2, and 3.4. For all of these modeling runs, minor constituents (from Ryan 1984) were included; nitrate was used to charge balance, sorption and mineral precipitation were ignored; and the system was open to the atmosphere (log fO_2 = -0.699 and log fCO_2 = -3.5).



Percentile	pH
10th percentile	2.7
25th percentile	2.9
median	3
75th percentile	3.2
90th percentile	3.4

* pH data include measurements from 1982-1990; seepage basins were capped ~ 1990.

Figure 9. pH in FSB78

3.4.4 Uncertainty

As shown by our modeling, the variability in pH in Basin 3 will not consist of large swings in pH or other geochemical parameters in response to short term oscillations in waste stream chemistry. Instead, Basin 3 chemistry would vary over a narrow range. We would expect that its chemistry would gradually drift from one condition to another in response to extended periods of different process campaigns in F Area. There are minimal data to support a specific explicit Basin 3 chemistry history; however statistics from the groundwater measurements from the core of the plume provide useful data for quantifying uncertainty.

Provided here is one example of how to apply the groundwater statistics for a UQ analysis. One could use the median Basin 3 chemistry (i.e., pH = 3 chemistry) as the base case. This base case would show results of using this one chemistry for the entire modeling period (e.g., 30 years). To evaluate sensitivity, this base case chemistry could then be varied annually using frequencies based on the FSB78 pH histogram. In other words, one could randomly select from the different conditions or parameters and vary the condition according to the observed probabilities or frequencies of FSB78. For example, if pH is selected as the condition to vary, one might randomly change it annually so that during the overall modeling period (e.g., 30 years) the chemistry has a pH of 2.7 for 15% of the time (e.g. 4 or 5 years), a pH of 2.9 for 15% of the time, a pH of 3.0 for 40% of the time (e.g., 12 years), a pH of 3.2 for 15% of the time and a pH of 3.4 for 15% of the time. By varying the chemistry on an annual basis (rather than a shorter timeframe), one would reasonably simulate a realistic slow shift between the various conditions. Comparing results from the sensitivity runs with the base case provides insight regarding the importance of the changes in specific parameter. If the variations do not make much difference in the simulation, then the nominal median charge balanced chemistry would be representative and there would be little need for additional UQ analysis on the particular parameter.

4.0 CONCLUSIONS

Results from this case study model for the F Area Seepage Basins provide data and understanding that can be used in further ASCEM modeling efforts of the F Area groundwater plume. As part of this modeling effort, we identify key geochemical factors that control overall basin water chemistry and the projected variability or stability. Key geochemical factors include the nature or chemistry of the waste streams, the open system of the basins, and duration of discharge of the types. Mixing models of the archetype waste streams indicated that the overall basin system would likely remain acidic much of the time. Only an extended period (perhaps a year or more) of alkaline waste discharge would dramatically alter the pH of the overall basin system.

Short term and long term variability were also evaluated by performing multiple stepwise modeling runs to calculate the oscillation of bulk chemistry in the basins in response to short term variations in waste stream chemistry. Short term (½ month and 1 month) oscillations in the waste stream types only affected the chemistry in Basin 1; little variation was observed in Basin 2 and 3. As the largest basin, Basin 3 is considered the primary source to the groundwater. As shown by our modeling, fluctuation in chemistry of the waste streams is not directly representative of the source term to the groundwater (i.e. Basin 3). The sequence of receiving basins and the large volume of water in Basin 3 "smooth" or nullify the short term variability in waste stream composition.

From our modeling and evaluation of groundwater data from the core of the plume, we developed a technically-based "charge-balanced" nominal source term chemistry for Basin 3 (Appendix E) over a narrow range of pH (2.7 to 3.4). We provide an example of how these data could be used to quantify uncertainty over the long term variations in waste stream chemistry and hence, Basin 3 chemistry.

5.0 REFERENCES

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APPENDIX A. SUMMARY TABLE MODEL RUNS

Basin	Fraction of Monthly Flow	Volume During Period (million L)	Inflow Type (Reactant)	Equivalent Flash Mix Ratio	Approximate Input pH	Basin pH (at specified flash mix ratio)
Scenario #1 -- 1/2 month duration waste streams						
Basin 1	0.25	3.25	generic acidic waste stream	0.565	2.5	2.7
	0.5	6.50	generic alkaline waste stream	0.811	12.0	8.0
	0.5	6.50	generic acidic waste stream	0.811	2.5	2.7
	0.5	6.50	generic alkaline waste stream	0.811	12.0	7.9
Basin 2	0.3865	5.02	generic acidic output from Basin 1	0.493	2.9	3.0
	0.227	2.95	generic basic output from Basin 1	0.329	7.7	3.2
	0.773	10.05	generic acidic output from Basin 1	0.743	2.9	3.0
	0.227	2.95	generic basic output from Basin 1	0.329	7.7	3.2
Basin 3	0.468	6.08	generic acidic output from Basin 2	0.108	3.0	3.0
	0.064	0.83	generic basic output from Basin 2	0.016	3.1	3.0
	0.936	12.17	generic acidic output from Basin 2	0.205	3.0	3.0
	0.064	0.83	generic basic output from Basin 2	0.016	3.1	3.0
	0.936	12.17	generic acidic output from Basin 2	0.205	3.0	3.0
	0.064	0.83	generic basic output from Basin 2	0.016	3.1	3.0
Scenario #2 -- 1 month duration waste streams						
Basin 1	1/2	6.50	generic acidic waste stream	0.811	2.5	2.6
	1	13.00	generic alkaline waste stream	0.964	12.0	8.2
	1	13.00	generic acidic waste stream	0.964	2.5	2.6
	1	13.00	generic alkaline waste stream	0.964	12.0	8.2
	1	13.00	generic acidic waste stream	0.964	2.5	2.6
Basin 2	0.64	8.32	generic acidic output from Basin 1	0.675	2.9	2.9
	0.72	9.36	generic basic output from Basin 1	0.718	7.9	3.4
	1.28	16.64	generic acidic output from Basin 1	0.894	2.9	2.9
	0.72	9.36	generic basic output from Basin 1	0.718	7.9	3.4
	1.28	16.64	generic acidic output from Basin 1	0.894	2.9	2.9
Basin 3	0.832	10.82	generic acidic output from Basin 2	0.185	3.0	3.0
	0.336	4.37	generic basic output from Basin 2	0.079	3.3	3.1
	1.664	21.63	generic acidic output from Basin 2	0.335	3.0	3.0
	0.336	4.37	generic basic output from Basin 2	0.079	3.3	3.0
	1.664	21.63	generic acidic output from Basin 2	0.335	3.0	3.0
	0.336	4.37	generic basic output from Basin 2	0.079	3.3	3.0

APPENDIX B. GWB OUTPUT FILES: ½ MONTH DISCHARGE DURATION

1) STARTING SOLUTION CHEMISTRY FOR BASIN 1

```
          Temperature =  25.0 C    Pressure =  1.013 bars
          pH =  3.044              log fO2 =   -0.699
          Eh =   1.0386 volts      pe =  17.5566
          Ionic strength      =    0.026462
          Activity of water   =    1.000000
          Solvent mass        =    1.000005 kg
          Solution mass       =    1.002218 kg
          Solution density    =    1.014    g/cm3
          Chlorinity          =    0.000000 molal
          Dissolved solids    =        2208 mg/kg sol'n
          Elect. conductivity =     2573.82 uS/cm (or umho/cm)
          Hardness            =       35.52 mg/kg sol'n as CaCO3
            carbonate         =        0.00 mg/kg sol'n as CaCO3
            non-carbonate     =       35.52 mg/kg sol'n as CaCO3
          Rock mass           =    0.000000 kg
          Carbonate alkalinity=        0.00 mg/kg sol'n as CaCO3
          Water type          =    Na-NO3
```

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			
Ca++	5.315e-005	5.315e-005	0.002130	
CaCO3	0.0003025	0.0003025	0.03028	
H+	4.418e-013	4.418e-013	4.453e-013	
H2O	27.75	27.75	500.0	
NO3-	0.0007169	0.0007169	0.04445	
Na+	0.008228	0.008228	0.1892	
O2(g)	-- fixed fugacity buffer --			
SiO2(aq)	4.521e-005	4.521e-005	0.002716	

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
NO3-	0.02614	1617.	0.8505	-1.6529
Na+	0.02444	560.7	0.8567	-1.6790
H+	0.001024	1.030	0.8813	-3.0444
Ca++	0.0003186	12.74	0.5625	-3.7466
O2(aq)	0.0002506	8.003	1.0069	-3.5980
SiO2(aq)	6.167e-005	3.697	1.0069	-4.2070
CaNO3+	3.709e-005	3.778	0.8567	-4.4980
CO2(aq)	1.116e-005	0.4900	1.0000	-4.9524

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Quartz	-0.2077	Cristobalite	-0.7582
Tridymite	-0.3735	Amrph^silica	-1.4934
Chalcedony	-0.4789		

```
    (only minerals with log Q/K > -3 listed)

  Gases                 fugacity      log fug.
 ------------------------------------------------
   O2(g)                   0.2000      -0.699
   Steam                  0.03131      -1.504
   CO2(g)               0.0003162      -3.500
   N2(g)                1.111e-005      -4.954
   H2(g)                6.282e-042     -41.202
   CH4(g)               3.888e-146    -145.410

                                    In fluid              Sorbed            Kd
  Original basis total moles   moles     mg/kg      moles     mg/kg      L/kg
 ------------------------------------------------------------------------------
--
   Ca++            0.000356   0.000356      14.2
   H+               0.00104    0.00104      1.04
   H2O                 55.5       55.5 9.98e+005
   HCO3-           1.12e-005  1.12e-005     0.680
   NO3-               0.0262     0.0262 1.62e+003
   Na+                0.0244     0.0244      561.
   O2(aq)          0.000251   0.000251      8.00
   SiO2(aq)        6.17e-005  6.17e-005      3.70
```

2) BASIN 1 CHEMISTRY AFTER ACIDIC WASTE STREAM, FLASH MIX RATIO=0.565

```
Step #   565             Xi = 0.5650
          Temperature =  25.0 C    Pressure =  1.013 bars
          pH =  2.701              log fO2 =   -0.699
          Eh =   1.0589 volts      pe =  17.9005
          Ionic strength      =    0.031626
          Activity of water   =    1.000000
          Solvent mass        =    1.000000 kg
          Solution mass       =    1.002638 kg
          Solution density    =    1.014    g/cm3
          Chlorinity          =    0.000000 molal
          Dissolved solids    =        2631 mg/kg sol'n
          Elect. conductivity =     3256.53 uS/cm (or umho/cm)
          Hardness            =       15.46 mg/kg sol'n as CaCO3
            carbonate         =        0.00 mg/kg sol'n as CaCO3
            non-carbonate     =       15.46 mg/kg sol'n as CaCO3
          Rock mass           =    0.000000 kg
          Carbonate alkalinity=        0.00 mg/kg sol'n as CaCO3
          Water type          =    Na-NO3

                           moles        moles         grams          cm3
  Reactants              remaining     reacted       reacted       reacted
 ------------------------------------------------------------------------------
   CO2(g)              -- fixed fugacity buffer --
   H+                    0.001409      0.001831      0.001845
   H2O                      24.15         31.36         565.0
   NO3-                   0.01553       0.02017         1.251
   Na+                    0.01409       0.01831        0.4209
   O2(g)               -- fixed fugacity buffer --
   SiO2(aq)            1.431e-005    1.859e-005      0.001117

  No minerals in system.
```

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
NO3-	0.03149	1947.	0.8399	-1.5776
Na+	0.02892	663.1	0.8470	-1.6109
H+	0.002278	2.290	0.8749	-2.7005
O2(aq)	0.0002503	7.989	1.0082	-3.5980
Ca++	0.0001365	5.456	0.5408	-4.1319
SiO2(aq)	4.543e-005	2.722	1.0082	-4.3391
CaNO3+	1.838e-005	1.871	0.8470	-4.8079
CO2(aq)	1.116e-005	0.4898	1.0000	-4.9524
N2(aq)	5.005e-008	0.001398	1.0000	-7.3006

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Quartz	-0.3398	Cristobalite	-0.8903
Tridymite	-0.5056	Amrph^silica	-1.6255
Chalcedony	-0.6110		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.2000	-0.699
Steam	0.03131	-1.504
CO2(g)	0.0003162	-3.500
N2(g)	7.660e-005	-4.116
H2(g)	6.282e-042	-41.202
CH4(g)	3.888e-146	-145.410

		In fluid		Sorbed		Kd
Original basis	total moles	moles	mg/kg	moles	mg/kg	L/kg
Ca++	0.000155	0.000155	6.19			
H+	0.00229	0.00229	2.30			
H2O	55.5	55.5	9.97e+005			
HCO3-	1.12e-005	1.12e-005	0.679			
NO3-	0.0315	0.0315	1.95e+003			
Na+	0.0289	0.0289	663.			
O2(aq)	0.000250	0.000250	7.98			
SiO2(aq)	4.54e-005	4.54e-005	2.72			

3) BASIN 1 CHEMISTRY AFTER ALKALINE WASTE STREAM, FLASH MIX RATIO=0.811

```
Step #   811             Xi = 0.8110
          Temperature =  25.0 C    Pressure =  1.013 bars
          pH =  7.980              log fO2 =   -0.699
          Eh =   0.7466 volts      pe =  12.6212
          Ionic strength      =    0.020510
          Activity of water   =    1.000000
          Solvent mass        =    0.999999 kg
          Solution mass       =    1.001710 kg
          Solution density    =    1.014    g/cm3
          Chlorinity          =    0.000000 molal
```

```
        Dissolved solids    =        1708 mg/kg sol'n
        Elect. conductivity =     1838.01 uS/cm (or umho/cm)
        Hardness            =       60.57 mg/kg sol'n as CaCO3
          carbonate         =       27.30 mg/kg sol'n as CaCO3
          non-carbonate     =       33.27 mg/kg sol'n as CaCO3
        Rock mass           =    0.000000 kg
        Carbonate alkalinity=       27.30 mg/kg sol'n as CaCO3
        Water type          =    Na-NO3
```

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			
Ca++	2.009e-005	8.620e-005	0.003455	
CaCO3	0.0001144	0.0004907	0.04911	
H+	1.670e-013	7.166e-013	7.223e-013	
H2O	10.49	45.02	811.0	
NO3-	0.0002710	0.001163	0.07210	
Na+	0.003110	0.01335	0.3068	
O2(g)	-- fixed fugacity buffer --			
SiO2(aq)	1.709e-005	7.333e-005	0.004406	

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
NO3-	0.01942	1202.	0.8648	-1.7748
Na+	0.01880	431.4	0.8699	-1.7864
Ca++	0.0005518	22.08	0.5934	-3.4849
HCO3-	0.0005257	32.02	0.8723	-3.3386
O2(aq)	0.0002510	8.019	1.0053	-3.5980
SiO2(aq)	8.025e-005	4.814	1.0053	-4.0932
CaNO3+	5.040e-005	5.136	0.8699	-4.3581
CO2(aq)	1.116e-005	0.4902	1.0000	-4.9524
NaHCO3	1.009e-005	0.8463	1.0000	-4.9961
CO3--	3.445e-006	0.2064	0.5756	-5.7028
CaHCO3+	2.859e-006	0.2886	0.8755	-5.6015
H3SiO4-	1.375e-006	0.1305	0.8699	-5.9223
OH-	1.134e-006	0.01926	0.8674	-6.0070
CaCO3	1.067e-006	0.1066	1.0000	-5.9717
NaH3SiO4	2.758e-007	0.03251	1.0000	-6.5594
NaCO3-	1.190e-007	0.009862	0.8699	-6.9849
H+	1.177e-008	1.184e-005	0.8904	-7.9798
NaOH	1.010e-008	0.0004032	1.0000	-7.9958

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Quartz	-0.0939	Cristobalite	-0.6444
Tridymite	-0.2597	Aragonite	-0.7216
Chalcedony	-0.3651	Amrph^silica	-1.3796
Calcite	-0.5567	Monohydrocalcite	-1.5506

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.

```
   O2(g)                    0.2000      -0.699
   Steam                   0.03131      -1.504
   CO2(g)                0.0003162      -3.500
   N2(g)                 8.535e-016     -15.069
   H2(g)                 6.282e-042     -41.202
   CH4(g)                3.888e-146    -145.410

                                    In fluid              Sorbed            Kd
  Original basis total moles   moles     mg/kg      moles     mg/kg      L/kg
 ----------------------------------------------------------------------------
---
   Ca++             0.000606   0.000606      24.3
   H+              3.73e-006  3.73e-006   0.00375
   H2O                  55.5       55.5 9.98e+005
   HCO3-            0.000554   0.000554      33.8
   NO3-               0.0195     0.0195 1.21e+003
   Na+                0.0188     0.0188      432.
   O2(aq)           0.000251   0.000251      8.02
   SiO2(aq)        8.19e-005  8.19e-005      4.91
```

4) BASIN 1 CHEMISTRY AFTER ACIDIC WASTE STREAM, FLASH MIX RATIO=0.811

```
Step #  8111             Xi = 0.8111
          Temperature =  25.0 C    Pressure =  1.013 bars
          pH =  2.657              log fO2 =   -0.699
          Eh =   1.0615 volts      pe =  17.9444
          Ionic strength      =    0.032670
          Activity of water   =    1.000000
          Solvent mass        =    1.000002 kg
          Solution mass       =    1.002726 kg
          Solution density    =    1.014    g/cm3
          Chlorinity          =    0.000000 molal
          Dissolved solids    =        2717 mg/kg sol'n
          Elect. conductivity =     3390.25 uS/cm (or umho/cm)
          Hardness            =       11.43 mg/kg sol'n as CaCO3
            carbonate         =        0.00 mg/kg sol'n as CaCO3
            non-carbonate     =       11.43 mg/kg sol'n as CaCO3
          Rock mass           =    0.000000 kg
          Carbonate alkalinity=        0.00 mg/kg sol'n as CaCO3
          Water type          =    Na-NO3

                           moles        moles         grams          cm3
  Reactants              remaining     reacted       reacted       reacted
 ----------------------------------------------------------------------------
   CO2(g)               -- fixed fugacity buffer --
   H+                    0.0006120      0.002628      0.002649
   H2O                       10.49         45.02         811.1
   NO3-                   0.006744       0.02896         1.795
   Na+                    0.006120       0.02628        0.6042
   O2(g)                -- fixed fugacity buffer --
   SiO2(aq)             6.215e-006    2.669e-005      0.001603

  No minerals in system.

  Aqueous species       molality    mg/kg sol'n    act. coef.     log act.
 ----------------------------------------------------------------------------
   NO3-                   0.03257         2014.      0.8379       -1.5640
```

```
   Na+                    0.02983         683.9      0.8452       -1.5984
   H+                    0.002524         2.537      0.8737       -2.6566
   O2(aq)               0.0002502         7.986      1.0085       -3.5980
   Ca++                 0.0001006         4.020      0.5368       -4.2677
   SiO2(aq)            4.216e-005         2.526      1.0085       -4.3715
   CaNO3+              1.390e-005         1.415      0.8452       -4.9300
   CO2(aq)             1.116e-005        0.4897      1.0000       -4.9524
   N2(aq)              6.523e-008      0.001822      1.0000       -7.1855
    (only species > 1e-8 molal listed)

  Mineral saturation states
                     log Q/K                              log Q/K
 ------------------------------------------------------------------
   Quartz            -0.3722        Cristobalite       -0.9227
   Tridymite         -0.5380        Amrph^silica       -1.6579
   Chalcedony        -0.6434
    (only minerals with log Q/K > -3 listed)

  Gases                fugacity      log fug.
 ------------------------------------------------
   O2(g)                  0.2000        -0.699
   Steam                 0.03131        -1.504
   CO2(g)              0.0003162        -3.500
   N2(g)               9.983e-005        -4.001
   H2(g)               6.282e-042       -41.202
   CH4(g)              3.888e-146       -145.410

                                    In fluid              Sorbed             Kd
  Original basis total moles   moles     mg/kg      moles     mg/kg      L/kg
 ------------------------------------------------------------------------------
---
   Ca++            0.000114   0.000114      4.58
   H+               0.00254    0.00254      2.55
   H2O                 55.5       55.5 9.97e+005
   HCO3-           1.12e-005  1.12e-005     0.679
   NO3-               0.0326     0.0326 2.01e+003
   Na+                0.0298     0.0298      684.
   O2(aq)           0.000250   0.000250      7.98
   SiO2(aq)        4.22e-005  4.22e-005      2.53
```

5) BASIN 1 CHEMISTRY AFTER ALKALINE WASTE STREAM, FLASH MIX RATIO=0.811

```
Step #   811             Xi = 0.8110
          Temperature =  25.0 C    Pressure =  1.013 bars
          pH =  7.941              log fO2 =   -0.699
          Eh =   0.7489 volts      pe =  12.6597
          Ionic strength      =    0.020658
          Activity of water   =    1.000000
          Solvent mass        =    1.000000 kg
          Solution mass       =    1.001724 kg
          Solution density    =    1.014    g/cm3
          Chlorinity          =    0.000000 molal
          Dissolved solids    =        1721 mg/kg sol'n
          Elect. conductivity =     1851.77 uS/cm (or umho/cm)
          Hardness            =       59.79 mg/kg sol'n as CaCO3
            carbonate         =       24.96 mg/kg sol'n as CaCO3
```

```
          non-carbonate     =       34.83 mg/kg sol'n as CaCO3
        Rock mass           =    0.000000 kg
        Carbonate alkalinity=       24.96 mg/kg sol'n as CaCO3
        Water type          =    Na-NO3
```

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			
Ca++	2.009e-005	8.620e-005	0.003455	
CaCO3	0.0001144	0.0004907	0.04911	
H+	1.670e-013	7.166e-013	7.223e-013	
H2O	10.49	45.02	811.0	
NO3-	0.0002710	0.001163	0.07210	
Na+	0.003110	0.01335	0.3068	
O2(g)	-- fixed fugacity buffer --			
SiO2(aq)	1.709e-005	7.333e-005	0.004406	

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
NO3-	0.01962	1215.	0.8644	-1.7705
Na+	0.01897	435.3	0.8695	-1.7827
Ca++	0.0005448	21.80	0.5925	-3.4911
HCO3-	0.0004812	29.31	0.8719	-3.3772
O2(aq)	0.0002510	8.018	1.0054	-3.5980
SiO2(aq)	7.979e-005	4.786	1.0054	-4.0957
CaNO3+	5.020e-005	5.116	0.8695	-4.3600
CO2(aq)	1.116e-005	0.4902	1.0000	-4.9524
NaHCO3	9.314e-006	0.7811	1.0000	-5.0308
CO3--	2.889e-006	0.1731	0.5746	-5.7798
CaHCO3+	2.580e-006	0.2604	0.8751	-5.6462
H3SiO4-	1.252e-006	0.1188	0.8695	-5.9633
OH-	1.039e-006	0.01763	0.8670	-6.0456
CaCO3	8.810e-007	0.08803	1.0000	-6.0550
NaH3SiO4	2.531e-007	0.02984	1.0000	-6.5967
NaCO3-	1.006e-007	0.008334	0.8695	-7.0582
H+	1.286e-008	1.294e-005	0.8902	-7.9412

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Quartz	-0.0964	Cristobalite	-0.6469
Tridymite	-0.2622	Aragonite	-0.8049
Chalcedony	-0.3676	Amrph^silica	-1.3821
Calcite	-0.6400	Monohydrocalcite	-1.6339

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.2000	-0.699
Steam	0.03131	-1.504
CO2(g)	0.0003162	-3.500
N2(g)	1.040e-015	-14.983
H2(g)	6.282e-042	-41.202

```
   CH4(g)              3.888e-146    -145.410

                                    In fluid              Sorbed            Kd
  Original basis total moles   moles     mg/kg      moles     mg/kg      L/kg
 ----------------------------------------------------------------------------
---
   Ca++            0.000598   0.000598      23.9
   H+             4.73e-006  4.73e-006   0.00476
   H2O                 55.5       55.5 9.98e+005
   HCO3-           0.000508   0.000508      31.0
   NO3-              0.0197     0.0197 1.22e+003
   Na+               0.0190     0.0190      436.
   O2(aq)          0.000251   0.000251      8.02
   SiO2(aq)       8.13e-005  8.13e-005      4.88
```

6) STARTING SOLUTION CHEMISTRY FOR BASIN 2

```
          Temperature =  25.0 C    Pressure =  1.013 bars
          pH =  3.044              log fO2 =   -0.699
          Eh =   1.0386 volts      pe =  17.5566
          Ionic strength      =    0.026462
          Activity of water   =    1.000000
          Solvent mass        =    1.000005 kg
          Solution mass       =    1.002218 kg
          Solution density    =    1.014    g/cm3
          Chlorinity          =    0.000000 molal
          Dissolved solids    =        2208 mg/kg sol'n
          Elect. conductivity =     2573.82 uS/cm (or umho/cm)
          Hardness            =       35.52 mg/kg sol'n as CaCO3
            carbonate         =        0.00 mg/kg sol'n as CaCO3
            non-carbonate     =       35.52 mg/kg sol'n as CaCO3
          Rock mass           =    0.000000 kg
          Carbonate alkalinity=        0.00 mg/kg sol'n as CaCO3
          Water type          =    Na-NO3

                          moles        moles         grams          cm3
  Reactants             remaining     reacted       reacted       reacted
 ----------------------------------------------------------------------------
   CO2(g)              -- fixed fugacity buffer --
   Ca++                5.315e-005    5.315e-005      0.002130
   CaCO3                0.0003025     0.0003025       0.03028
   H+                  4.418e-013    4.418e-013    4.453e-013
   H2O                      27.75         27.75         500.0
   NO3-                 0.0007169     0.0007169       0.04445
   Na+                   0.008228      0.008228        0.1892
   O2(g)               -- fixed fugacity buffer --
   SiO2(aq)            4.521e-005    4.521e-005      0.002716

  No minerals in system.

  Aqueous species       molality    mg/kg sol'n    act. coef.     log act.
 ----------------------------------------------------------------------------
   NO3-                   0.02614         1617.      0.8505       -1.6529
   Na+                    0.02444         560.7      0.8567       -1.6790
   H+                    0.001024         1.030      0.8813       -3.0444
   Ca++                 0.0003186         12.74      0.5625       -3.7466
   O2(aq)               0.0002506         8.003      1.0069       -3.5980
```

```
   SiO2(aq)            6.167e-005         3.697      1.0069       -4.2070
   CaNO3+              3.709e-005         3.778      0.8567       -4.4980
   CO2(aq)             1.116e-005        0.4900      1.0000       -4.9524
    (only species > 1e-8 molal listed)

  Mineral saturation states
                     log Q/K                              log Q/K
 ------------------------------------------------------------------
   Quartz            -0.2077        Cristobalite       -0.7582
   Tridymite         -0.3735        Amrph^silica       -1.4934
   Chalcedony        -0.4789
    (only minerals with log Q/K > -3 listed)

  Gases                 fugacity      log fug.
 ------------------------------------------------
   O2(g)                    0.2000      -0.699
   Steam                   0.03131      -1.504
   CO2(g)                0.0003162      -3.500
   N2(g)                1.111e-005      -4.954
   H2(g)                6.282e-042     -41.202
   CH4(g)               3.888e-146    -145.410

                                    In fluid              Sorbed             Kd
  Original basis total moles   moles     mg/kg      moles     mg/kg       L/kg
 ------------------------------------------------------------------------------
---
   Ca++             0.000356   0.000356      14.2
   H+                0.00104    0.00104      1.04
   H2O                  55.5       55.5 9.98e+005
   HCO3-            1.12e-005  1.12e-005     0.680
   NO3-                0.0262     0.0262 1.62e+003
   Na+                 0.0244     0.0244      561.
   O2(aq)            0.000251   0.000251      8.00
   SiO2(aq)         6.17e-005  6.17e-005      3.70
```

7) BASIN 2 CHEMISTRY AFTER ACIDIC DISCHARGE FROM BASIN 1, FLASH MIX RATIO=0.493

```
   Step #   493             Xi = 0.4930
          Temperature =  25.0 C    Pressure =  1.013 bars
          pH =  2.992              log fO2 =   -0.699
          Eh =   1.0417 volts      pe =  17.6093
          Ionic strength      =    0.026936
          Activity of water   =    1.000000
          Solvent mass        =    1.000000 kg
          Solution mass       =    1.002252 kg
          Solution density    =    1.014    g/cm3
          Chlorinity          =    0.000000 molal
          Dissolved solids    =        2247 mg/kg sol'n
          Elect. conductivity =     2641.62 uS/cm (or umho/cm)
          Hardness            =       33.48 mg/kg sol'n as CaCO3
            carbonate         =        0.00 mg/kg sol'n as CaCO3
            non-carbonate     =       33.48 mg/kg sol'n as CaCO3
          Rock mass           =    0.000000 kg
          Carbonate alkalinity=        0.00 mg/kg sol'n as CaCO3
          Water type          =    Na-NO3
```

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			
Ca++	0.0001592	0.0001548	0.006204	
H+	0.0006540	0.0006360	0.0006410	
H2O	28.14	27.37	493.0	
NO3-	0.01379	0.01341	0.8315	
Na+	0.01283	0.01247	0.2867	
O2(g)	-- fixed fugacity buffer --			
SiO2(aq)	2.961e-005	2.879e-005	0.001730	

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
NO3-	0.02664	1648.	0.8495	-1.6454
Na+	0.02484	569.9	0.8558	-1.6724
H+	0.001158	1.164	0.8807	-2.9916
Ca++	0.0002999	11.99	0.5604	-3.7746
O2(aq)	0.0002506	8.001	1.0070	-3.5980
SiO2(aq)	6.007e-005	3.601	1.0070	-4.2183
CaNO3+	3.542e-005	3.608	0.8558	-4.5183
CO2(aq)	1.116e-005	0.4900	1.0000	-4.9524

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Quartz	-0.2190	Cristobalite	-0.7695
Tridymite	-0.3848	Amrph^silica	-1.5047
Chalcedony	-0.4902		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.2000	-0.699
Steam	0.03131	-1.504
CO2(g)	0.0003162	-3.500
N2(g)	1.467e-005	-4.834
H2(g)	6.282e-042	-41.202
CH4(g)	3.888e-146	-145.410

Original basis	total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg	Kd L/kg
Ca++	0.000335	0.000335	13.4			
H+	0.00117	0.00117	1.18			
H2O	55.5	55.5	9.98e+005			
HCO3-	1.12e-005	1.12e-005	0.680			
NO3-	0.0267	0.0267	1.65e+003			
Na+	0.0248	0.0248	570.			
O2(aq)	0.000251	0.000251	8.00			
SiO2(aq)	6.01e-005	6.01e-005	3.60			

8) BASIN 2 CHEMISTRY AFTER ALKALINE DISCHARGE FROM BASIN 1, FLASH MIX RATIO=0.329

```
       Step #   329             Xi = 0.3290
          Temperature =  25.0 C    Pressure =  1.013 bars
          pH =  3.162              log fO2 =   -0.699
          Eh =   1.0316 volts      pe =  17.4394
          Ionic strength      =    0.025082
          Activity of water   =    1.000000
          Solvent mass        =    1.000000 kg
          Solution mass       =    1.002097 kg
          Solution density    =    1.014    g/cm3
          Chlorinity          =    0.000000 molal
          Dissolved solids    =        2093 mg/kg sol'n
          Elect. conductivity =     2407.51 uS/cm (or umho/cm)
          Hardness            =       40.92 mg/kg sol'n as CaCO3
            carbonate         =        0.00 mg/kg sol'n as CaCO3
            non-carbonate     =       40.92 mg/kg sol'n as CaCO3
          Rock mass           =    0.000000 kg
          Carbonate alkalinity=        0.00 mg/kg sol'n as CaCO3
          Water type          =    Na-NO3
```

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			
Ca++	0.0003771	0.0001849	0.007411	
H+	5.791e-006	2.839e-006	2.862e-006	
H2O	37.25	18.26	329.0	
NO3-	0.01382	0.006777	0.4202	
Na+	0.01329	0.006514	0.1498	
O2(g)	-- fixed fugacity buffer --			
SiO2(aq)	5.261e-005	2.579e-005	0.001550	

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
NO3-	0.02471	1529.	0.8536	-1.6758
Na+	0.02315	531.2	0.8595	-1.7011
H+	0.0007804	0.7849	0.8833	-3.1616
Ca++	0.0003686	14.74	0.5691	-3.6782
O2(aq)	0.0002507	8.006	1.0065	-3.5980
SiO2(aq)	6.612e-005	3.965	1.0065	-4.1768
CaNO3+	4.105e-005	4.182	0.8595	-4.4524
CO2(aq)	1.116e-005	0.4900	1.0000	-4.9524

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Quartz	-0.1775	Cristobalite	-0.7280
Tridymite	-0.3433	Amrph^silica	-1.4632
Chalcedony	-0.4487		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.

O2(g)	0.2000	-0.699
Steam	0.03131	-1.504
CO2(g)	0.0003162	-3.500
N2(g)	5.830e-006	-5.234
H2(g)	6.282e-042	-41.202
CH4(g)	3.888e-146	-145.410

9) BASIN 2 CHEMISTRY AFTER ACIDIC DISCHARGE FROM BASIN 1, FLASH MIX RATIO=0.743

Step # 743 Xi = 0.7430

Temperature =	25.0 C	Pressure =	1.013 bars
pH =	2.991	log fO2 =	-0.699
Eh =	1.0417 volts	pe =	17.6100
Ionic strength	=	0.026864	
Activity of water	=	1.000000	
Solvent mass	=	1.000000 kg	
Solution mass	=	1.002245 kg	
Solution density	=	1.014 g/cm3	
Chlorinity	=	0.000000 molal	
Dissolved solids	=	2240 mg/kg sol'n	
Elect. conductivity	=	2636.11 uS/cm (or umho/cm)	
Hardness	=	33.82 mg/kg sol'n as CaCO3	
carbonate	=	0.00 mg/kg sol'n as CaCO3	
non-carbonate	=	33.82 mg/kg sol'n as CaCO3	
Rock mass	=	0.000000 kg	
Carbonate alkalinity	=	0.00 mg/kg sol'n as CaCO3	
Water type	=	Na-NO3	

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			
Ca++	8.070e-005	0.0002333	0.009351	
H+	0.0003315	0.0009585	0.0009660	
H2O	14.27	41.24	743.0	
NO3-	0.006990	0.02021	1.253	
Na+	0.006502	0.01880	0.4322	
O2(g)	-- fixed fugacity buffer --			
SiO2(aq)	1.501e-005	4.339e-005	0.002607	

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
NO3-	0.02656	1643.	0.8497	-1.6465
Na+	0.02476	568.0	0.8559	-1.6738
H+	0.001159	1.166	0.8808	-2.9910
Ca++	0.0003030	12.12	0.5607	-3.7699
O2(aq)	0.0002506	8.001	1.0070	-3.5980
SiO2(aq)	6.038e-005	3.620	1.0070	-4.2161
CaNO3+	3.571e-005	3.637	0.8559	-4.5148
CO2(aq)	1.116e-005	0.4900	1.0000	-4.9524

(only species > 1e-8 molal listed)

Mineral saturation states

```
                    log Q/K                              log Q/K
 ------------------------------------------------------------------
   Quartz            -0.2168        Cristobalite      -0.7673
   Tridymite         -0.3826        Amrph^silica      -1.5025
   Chalcedony        -0.4880
    (only minerals with log Q/K > -3 listed)

  Gases                fugacity      log fug.
 ------------------------------------------------
   O2(g)                   0.2000      -0.699
   Steam                  0.03131      -1.504
   CO2(g)               0.0003162      -3.500
   N2(g)                1.464e-005      -4.835
   H2(g)                6.282e-042     -41.202
   CH4(g)               3.888e-146    -145.410

                                  In fluid              Sorbed             Kd
  Original basis total moles   moles     mg/kg      moles     mg/kg      L/kg
 ------------------------------------------------------------------------------
---
   Ca++            0.000339   0.000339      13.5
   H+               0.00117    0.00117      1.18
   H2O                 55.5       55.5 9.98e+005
   HCO3-           1.12e-005  1.12e-005     0.680
   NO3-               0.0266     0.0266 1.65e+003
   Na+                0.0248     0.0248      568.
   O2(aq)           0.000251   0.000251      8.00
   SiO2(aq)        6.04e-005  6.04e-005      3.62
```

10) BASIN 2 CHEMISTRY AFTER ALKALINE DISCHARGE FROM BASIN 1, FLASH MIX RATIO=0.329

```
      Step #   329             Xi = 0.3290
          Temperature =  25.0 C    Pressure =  1.013 bars
          pH =  3.162              log fO2 =   -0.699
          Eh =   1.0316 volts      pe =  17.4394
          Ionic strength      =    0.025090
          Activity of water   =    1.000000
          Solvent mass        =    1.000000 kg
          Solution mass       =    1.002097 kg
          Solution density    =    1.014    g/cm3
          Chlorinity          =    0.000000 molal
          Dissolved solids    =        2093 mg/kg sol'n
          Elect. conductivity =     2407.91 uS/cm (or umho/cm)
          Hardness            =       41.19 mg/kg sol'n as CaCO3
            carbonate         =        0.00 mg/kg sol'n as CaCO3
            non-carbonate     =       41.19 mg/kg sol'n as CaCO3
          Rock mass           =    0.000000 kg
          Carbonate alkalinity=        0.00 mg/kg sol'n as CaCO3
          Water type          =    Na-NO3

                           moles        moles         grams          cm3
  Reactants              remaining     reacted       reacted       reacted
 ------------------------------------------------------------------------------
   CO2(g)               -- fixed fugacity buffer --
   Ca++                  0.0003771     0.0001849      0.007411
   H+                   5.791e-006    2.839e-006    2.862e-006
```

```
  H2O                    37.25         18.26         329.0
  NO3-                 0.01382      0.006777        0.4202
  Na+                  0.01329      0.006514        0.1498
  O2(g)             -- fixed fugacity buffer --
  SiO2(aq)          5.261e-005    2.579e-005      0.001550

 No minerals in system.

 Aqueous species       molality    mg/kg sol'n    act. coef.     log act.
-------------------------------------------------------------------------
  NO3-                 0.02472         1529.      0.8536       -1.6757
  Na+                  0.02315         531.2      0.8595       -1.7011
  H+                  0.0007804        0.7849      0.8833       -3.1616
  Ca++                0.0003710         14.84      0.5690       -3.6754
  O2(aq)              0.0002507         8.006      1.0065       -3.5980
  SiO2(aq)           6.632e-005         3.977      1.0065       -4.1755
  CaNO3+             4.132e-005         4.210      0.8595       -4.4496
  CO2(aq)            1.116e-005        0.4900      1.0000       -4.9524
   (only species > 1e-8 molal listed)

 Mineral saturation states
                   log Q/K                              log Q/K
-----------------------------------------------------------------
  Quartz           -0.1762        Cristobalite        -0.7267
  Tridymite        -0.3420        Amrph^silica        -1.4619
  Chalcedony       -0.4474
   (only minerals with log Q/K > -3 listed)

 Gases                fugacity      log fug.
------------------------------------------------
  O2(g)                 0.2000        -0.699
  Steam                0.03131        -1.504
  CO2(g)             0.0003162        -3.500
  N2(g)              5.832e-006        -5.234
  H2(g)              6.282e-042       -41.202
  CH4(g)             3.888e-146      -145.410

                                 In fluid              Sorbed            Kd
 Original basis total moles    moles     mg/kg      moles     mg/kg      L/kg
-------------------------------------------------------------------------------
---
  Ca++            0.000412   0.000412      16.5
  H+              0.000792   0.000792     0.796
  H2O                55.5       55.5 9.98e+005
  HCO3-          1.12e-005  1.12e-005     0.680
  NO3-              0.0248     0.0248 1.53e+003
  Na+               0.0232     0.0232      531.
  O2(aq)          0.000251   0.000251      8.01
  SiO2(aq)       6.63e-005  6.63e-005      3.98
```

11) STARTING SOLUTION CHEMISTRY FOR BASIN 3

```
          Temperature =  25.0 C    Pressure =  1.013 bars
          pH =  3.044              log fO2 =   -0.699
          Eh =   1.0386 volts      pe =  17.5566
          Ionic strength      =    0.026462
```

```
        Activity of water   =    1.000000
        Solvent mass        =    1.000005 kg
        Solution mass       =    1.002218 kg
        Solution density    =    1.014    g/cm3
        Chlorinity          =    0.000000 molal
        Dissolved solids    =        2208 mg/kg sol'n
        Elect. conductivity =     2573.82 uS/cm (or umho/cm)
        Hardness            =       35.52 mg/kg sol'n as CaCO3
          carbonate         =        0.00 mg/kg sol'n as CaCO3
          non-carbonate     =       35.52 mg/kg sol'n as CaCO3
        Rock mass           =    0.000000 kg
        Carbonate alkalinity=        0.00 mg/kg sol'n as CaCO3
        Water type          =    Na-NO3
```

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			
Ca++	5.315e-005	5.315e-005	0.002130	
CaCO3	0.0003025	0.0003025	0.03028	
H+	4.418e-013	4.418e-013	4.453e-013	
H2O	27.75	27.75	500.0	
NO3-	0.0007169	0.0007169	0.04445	
Na+	0.008228	0.008228	0.1892	
O2(g)	-- fixed fugacity buffer --			
SiO2(aq)	4.521e-005	4.521e-005	0.002716	

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
NO3-	0.02614	1617.	0.8505	-1.6529
Na+	0.02444	560.7	0.8567	-1.6790
H+	0.001024	1.030	0.8813	-3.0444
Ca++	0.0003186	12.74	0.5625	-3.7466
O2(aq)	0.0002506	8.003	1.0069	-3.5980
SiO2(aq)	6.167e-005	3.697	1.0069	-4.2070
CaNO3+	3.709e-005	3.778	0.8567	-4.4980
CO2(aq)	1.116e-005	0.4900	1.0000	-4.9524

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Quartz	-0.2077	Cristobalite	-0.7582
Tridymite	-0.3735	Amrph^silica	-1.4934
Chalcedony	-0.4789		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.2000	-0.699
Steam	0.03131	-1.504
CO2(g)	0.0003162	-3.500
N2(g)	1.111e-005	-4.954
H2(g)	6.282e-042	-41.202
CH4(g)	3.888e-146	-145.410

Original basis	total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg	Kd L/kg
Ca++	0.000356	0.000356	14.2			
H+	0.00104	0.00104	1.04			
H2O	55.5	55.5	9.98e+005			
HCO3-	1.12e-005	1.12e-005	0.680			
NO3-	0.0262	0.0262	1.62e+003			
Na+	0.0244	0.0244	561.			
O2(aq)	0.000251	0.000251	8.00			
SiO2(aq)	6.17e-005	6.17e-005	3.70			

12) BASIN 3 CHEMISTRY AFTER ACIDIC DISCHARGE FROM BASIN 2, FLASH MIX RATIO=0.108

Step # 108 Xi = 0.1080
Temperature = 25.0 C Pressure = 1.013 bars
pH = 3.038 log fO2 = -0.699
Eh = 1.0389 volts pe = 17.5626
Ionic strength = 0.026451
Activity of water = 1.000000
Solvent mass = 1.000000 kg
Solution mass = 1.002212 kg
Solution density = 1.014 g/cm3
Chlorinity = 0.000000 molal
Dissolved solids = 2207 mg/kg sol'n
Elect. conductivity = 2576.14 uS/cm (or umho/cm)
Hardness = 35.43 mg/kg sol'n as CaCO3
carbonate = 0.00 mg/kg sol'n as CaCO3
non-carbonate = 35.43 mg/kg sol'n as CaCO3
Rock mass = 0.000000 kg
Carbonate alkalinity= 0.00 mg/kg sol'n as CaCO3
Water type = Na-NO3

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			
Ca++	0.0003077	3.726e-005	0.001493	
H+	0.0009990	0.0001210	0.0001219	
H2O	49.51	5.995	108.0	
NO3-	0.02355	0.002851	0.1768	
Na+	0.02194	0.002657	0.06108	
O2(g)	-- fixed fugacity buffer --			
SiO2(aq)	5.432e-005	6.577e-006	0.0003952	

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
NO3-	0.02613	1617.	0.8506	-1.6531
Na+	0.02442	560.2	0.8567	-1.6794
H+	0.001039	1.045	0.8814	-3.0384
Ca++	0.0003178	12.71	0.5626	-3.7476
O2(aq)	0.0002506	8.003	1.0069	-3.5980

```
   SiO2(aq)            6.161e-005         3.694      1.0069       -4.2073
   CaNO3+              3.699e-005         3.767      0.8567       -4.4991
   CO2(aq)             1.116e-005        0.4900      1.0000       -4.9524
    (only species > 1e-8 molal listed)

  Mineral saturation states
                     log Q/K                              log Q/K
 ------------------------------------------------------------------
   Quartz            -0.2080        Cristobalite       -0.7585
   Tridymite         -0.3738        Amrph^silica       -1.4937
   Chalcedony        -0.4792
    (only minerals with log Q/K > -3 listed)

  Gases                 fugacity      log fug.
 ------------------------------------------------
   O2(g)                    0.2000      -0.699
   Steam                   0.03131      -1.504
   CO2(g)                0.0003162      -3.500
   N2(g)                1.141e-005      -4.943
   H2(g)                6.282e-042     -41.202
   CH4(g)               3.888e-146    -145.410

                                    In fluid              Sorbed             Kd
  Original basis total moles   moles     mg/kg      moles     mg/kg       L/kg
 ------------------------------------------------------------------------------
---
   Ca++             0.000355   0.000355      14.2
   H+                0.00105    0.00105      1.06
   H2O                  55.5       55.5 9.98e+005
   HCO3-            1.12e-005  1.12e-005     0.680
   NO3-                0.0262     0.0262 1.62e+003
   Na+                 0.0244     0.0244      560.
   O2(aq)            0.000251   0.000251      8.00
   SiO2(aq)         6.16e-005  6.16e-005      3.69
```

13) BASIN 3 CHEMISTRY AFTER ALKALINE DISCHARGE FROM BASIN 2, FLASH MIX RATIO=0.016

```
       Step #    16             Xi = 0.0160
          Temperature =  25.0 C    Pressure =  1.013 bars
          pH =  3.045              log fO2 =   -0.699
          Eh =   1.0385 volts      pe =  17.5557
          Ionic strength      =    0.026401
          Activity of water   =    1.000000
          Solvent mass        =    1.000000 kg
          Solution mass       =    1.002208 kg
          Solution density    =    1.014    g/cm3
          Chlorinity          =    0.000000 molal
          Dissolved solids    =        2203 mg/kg sol'n
          Elect. conductivity =     2568.58 uS/cm (or umho/cm)
          Hardness            =       35.52 mg/kg sol'n as CaCO3
            carbonate         =        0.00 mg/kg sol'n as CaCO3
            non-carbonate     =       35.52 mg/kg sol'n as CaCO3
          Rock mass           =    0.000000 kg
          Carbonate alkalinity=        0.00 mg/kg sol'n as CaCO3
          Water type          =    Na-NO3
```

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			
Ca++	0.0003897	6.336e-006	0.0002539	
H+	8.472e-006	1.378e-007	1.388e-007	
H2O	54.62	0.8881	16.00	
NO3-	0.02470	0.0004016	0.02490	
Na+	0.02312	0.0003760	0.008644	
O2(g)	-- fixed fugacity buffer --			
SiO2(aq)	6.396e-005	1.040e-006	6.249e-005	

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
NO3-	0.02608	1614.	0.8507	-1.6539
Na+	0.02439	559.4	0.8568	-1.6800
H+	0.001022	1.028	0.8814	-3.0452
Ca++	0.0003186	12.74	0.5628	-3.7463
O2(aq)	0.0002506	8.003	1.0069	-3.5980
SiO2(aq)	6.165e-005	3.696	1.0069	-4.2071
CaNO3+	3.702e-005	3.771	0.8568	-4.4986
CO2(aq)	1.116e-005	0.4900	1.0000	-4.9524

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Quartz	-0.2078	Cristobalite	-0.7583
Tridymite	-0.3736	Amrph^silica	-1.4935
Chalcedony	-0.4790		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.2000	-0.699
Steam	0.03131	-1.504
CO2(g)	0.0003162	-3.500
N2(g)	1.102e-005	-4.958
H2(g)	6.282e-042	-41.202
CH4(g)	3.888e-146	-145.410

Original basis total moles	In fluid moles	In fluid mg/kg	Sorbed moles	Sorbed mg/kg	Kd L/kg
Ca++	0.000356	0.000356	14.2		
H+	0.00103	0.00103	1.04		
H2O	55.5	55.5	9.98e+005		
HCO3-	1.12e-005	1.12e-005	0.680		
NO3-	0.0261	0.0261	1.62e+003		
Na+	0.0244	0.0244	559.		
O2(aq)	0.000251	0.000251	8.00		
SiO2(aq)	6.17e-005	6.17e-005	3.70		

14) BASIN 3 CHEMISTRY AFTER ACIDIC DISCHARGE FROM BASIN 2, FLASH MIX RATIO=0.205

```
        Step #   205             Xi = 0.2050
          Temperature =  25.0 C    Pressure =  1.013 bars
          pH =  3.038              log fO2 =   -0.699
          Eh =   1.0389 volts      pe =  17.5629
          Ionic strength      =    0.026468
          Activity of water   =    1.000000
          Solvent mass        =    1.000000 kg
          Solution mass       =    1.002213 kg
          Solution density    =    1.014    g/cm3
          Chlorinity          =    0.000000 molal
          Dissolved solids    =        2208 mg/kg sol'n
          Elect. conductivity =     2577.77 uS/cm (or umho/cm)
          Hardness            =       35.33 mg/kg sol'n as CaCO3
            carbonate         =        0.00 mg/kg sol'n as CaCO3
            non-carbonate     =       35.33 mg/kg sol'n as CaCO3
          Rock mass           =    0.000000 kg
          Carbonate alkalinity=        0.00 mg/kg sol'n as CaCO3
          Water type          =    Na-NO3
```

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			
Ca++	0.0002743	7.073e-005	0.002835	
H+	0.0008904	0.0002296	0.0002314	
H2O	44.13	11.38	205.0	
NO3-	0.02099	0.005412	0.3356	
Na+	0.01956	0.005043	0.1159	
O2(g)	-- fixed fugacity buffer --			
SiO2(aq)	4.842e-005	1.248e-005	0.0007501	

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
NO3-	0.02615	1618.	0.8505	-1.6528
Na+	0.02444	560.7	0.8567	-1.6791
H+	0.001040	1.045	0.8813	-3.0380
Ca++	0.0003169	12.67	0.5625	-3.7490
O2(aq)	0.0002506	8.003	1.0069	-3.5980
SiO2(aq)	6.154e-005	3.689	1.0069	-4.2079
CaNO3+	3.689e-005	3.758	0.8567	-4.5002
CO2(aq)	1.116e-005	0.4900	1.0000	-4.9524

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Quartz	-0.2086	Cristobalite	-0.7591
Tridymite	-0.3744	Amrph^silica	-1.4943
Chalcedony	-0.4798		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.2000	-0.699
Steam	0.03131	-1.504
CO2(g)	0.0003162	-3.500
N2(g)	1.145e-005	-4.941
H2(g)	6.282e-042	-41.202
CH4(g)	3.888e-146	-145.410

		In fluid		Sorbed		Kd
Original basis	total moles	moles	mg/kg	moles	mg/kg	L/kg
Ca++	0.000354	0.000354	14.1			
H+	0.00105	0.00105	1.06			
H2O	55.5	55.5	9.98e+005			
HCO3-	1.12e-005	1.12e-005	0.680			
NO3-	0.0262	0.0262	1.62e+003			
Na+	0.0244	0.0244	561.			
O2(aq)	0.000251	0.000251	8.00			
SiO2(aq)	6.15e-005	6.15e-005	3.69			

15) BASIN 3 CHEMISTRY AFTER ALKALINE DISCHARGE FROM BASIN 2, FLASH MIX RATIO=0.016

Step # 16 Xi = 0.0160
Temperature = 25.0 C Pressure = 1.013 bars
pH = 3.045 log fO2 = -0.699
Eh = 1.0385 volts pe = 17.5557
Ionic strength = 0.026398
Activity of water = 1.000000
Solvent mass = 1.000000 kg
Solution mass = 1.002207 kg
Solution density = 1.014 g/cm3
Chlorinity = 0.000000 molal
Dissolved solids = 2203 mg/kg sol'n
Elect. conductivity = 2568.43 uS/cm (or umho/cm)
Hardness = 35.42 mg/kg sol'n as CaCO3
carbonate = 0.00 mg/kg sol'n as CaCO3
non-carbonate = 35.42 mg/kg sol'n as CaCO3
Rock mass = 0.000000 kg
Carbonate alkalinity= 0.00 mg/kg sol'n as CaCO3
Water type = Na-NO3

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			
Ca++	0.0003897	6.336e-006	0.0002539	
H+	8.472e-006	1.378e-007	1.388e-007	
H2O	54.62	0.8881	16.00	
NO3-	0.02470	0.0004016	0.02490	
Na+	0.02312	0.0003760	0.008644	
O2(g)	-- fixed fugacity buffer --			
SiO2(aq)	6.396e-005	1.040e-006	6.249e-005	

```
 No minerals in system.

 Aqueous species       molality    mg/kg sol'n    act. coef.     log act.
-------------------------------------------------------------------------
  NO3-                  0.02608         1614.      0.8507       -1.6539
  Na+                   0.02439         559.4      0.8568       -1.6800
  H+                   0.001022         1.028      0.8814       -3.0452
  Ca++                 0.0003178         12.71      0.5628       -3.7475
  O2(aq)               0.0002506         8.003      1.0069       -3.5980
  SiO2(aq)            6.156e-005         3.690      1.0069       -4.2078
  CaNO3+              3.692e-005         3.761      0.8568       -4.4998
  CO2(aq)             1.116e-005        0.4900      1.0000       -4.9524
   (only species > 1e-8 molal listed)

 Mineral saturation states
                    log Q/K                              log Q/K
-----------------------------------------------------------------
  Quartz            -0.2085       Cristobalite         -0.7590
  Tridymite         -0.3743       Amrph^silica         -1.4942
  Chalcedony        -0.4797
   (only minerals with log Q/K > -3 listed)

 Gases                fugacity      log fug.
-----------------------------------------------
  O2(g)                  0.2000        -0.699
  Steam                 0.03131        -1.504
  CO2(g)               0.0003162        -3.500
  N2(g)               1.102e-005        -4.958
  H2(g)               6.282e-042       -41.202
  CH4(g)              3.888e-146      -145.410

                                  In fluid              Sorbed             Kd
 Original basis total moles   moles     mg/kg      moles     mg/kg       L/kg
-------------------------------------------------------------------------------
---
  Ca++            0.000355   0.000355      14.2
  H+               0.00103    0.00103      1.04
  H2O                 55.5       55.5 9.98e+005
  HCO3-          1.12e-005  1.12e-005     0.680
  NO3-              0.0261     0.0261 1.62e+003
  Na+               0.0244     0.0244      559.
  O2(aq)          0.000251   0.000251      8.00
  SiO2(aq)       6.16e-005  6.16e-005      3.69
```

16) BASIN 3 CHEMISTRY AFTER ACIDIC DISCHARGE FROM BASIN 2, FLASH MIX RATIO=0.205

```
     Step #   205             Xi = 0.2050
          Temperature =  25.0 C    Pressure =  1.013 bars
          pH =  3.038              log fO2 =   -0.699
          Eh =   1.0389 volts      pe =  17.5629
          Ionic strength      =    0.026466
          Activity of water   =    1.000000
          Solvent mass        =    1.000000 kg
          Solution mass       =    1.002213 kg
          Solution density    =    1.014    g/cm3
          Chlorinity          =    0.000000 molal
```

```
          Dissolved solids    =        2208 mg/kg sol'n
          Elect. conductivity =     2577.65 uS/cm (or umho/cm)
          Hardness            =       35.25 mg/kg sol'n as CaCO3
            carbonate         =        0.00 mg/kg sol'n as CaCO3
            non-carbonate     =       35.25 mg/kg sol'n as CaCO3
          Rock mass           =    0.000000 kg
          Carbonate alkalinity=        0.00 mg/kg sol'n as CaCO3
          Water type          =    Na-NO3

                          moles        moles         grams          cm3
 Reactants              remaining     reacted       reacted       reacted
-------------------------------------------------------------------------
  CO2(g)               -- fixed fugacity buffer --
  Ca++                  0.0002743    7.073e-005      0.002835
  H+                    0.0008904     0.0002296     0.0002314
  H2O                       44.13         11.38         205.0
  NO3-                    0.02099      0.005412        0.3356
  Na+                     0.01956      0.005043        0.1159
  O2(g)                -- fixed fugacity buffer --
  SiO2(aq)             4.842e-005    1.248e-005     0.0007501

 No minerals in system.

 Aqueous species       molality    mg/kg sol'n    act. coef.     log act.
-------------------------------------------------------------------------
  NO3-                   0.02615         1618.      0.8505       -1.6528
  Na+                    0.02444         560.7      0.8567       -1.6791
  H+                    0.001040         1.045      0.8813       -3.0380
  Ca++                  0.0003161         12.64      0.5625       -3.7500
  O2(aq)                0.0002506         8.003      1.0069       -3.5980
  SiO2(aq)             6.146e-005         3.684      1.0069       -4.2085
  CaNO3+               3.681e-005         3.749      0.8567       -4.5012
  CO2(aq)              1.116e-005        0.4900      1.0000       -4.9524
   (only species > 1e-8 molal listed)

 Mineral saturation states
                    log Q/K                            log Q/K
-------------------------------------------------------------------
  Quartz            -0.2092        Cristobalite       -0.7597
  Tridymite         -0.3750        Amrph^silica       -1.4949
  Chalcedony        -0.4804
   (only minerals with log Q/K > -3 listed)

 Gases                 fugacity      log fug.
-------------------------------------------------
  O2(g)                   0.2000       -0.699
  Steam                  0.03131       -1.504
  CO2(g)                0.0003162       -3.500
  N2(g)                1.145e-005       -4.941
  H2(g)                6.282e-042      -41.202
  CH4(g)               3.888e-146     -145.410

                                  In fluid              Sorbed             Kd
 Original basis total moles   moles     mg/kg      moles     mg/kg      L/kg
-------------------------------------------------------------------------------
---
  Ca++            0.000353   0.000353      14.1
```

```
  H+               0.00105    0.00105      1.06
  H2O                 55.5       55.5 9.98e+005
  HCO3-           1.12e-005  1.12e-005     0.680
  NO3-               0.0262     0.0262 1.62e+003
  Na+                0.0244     0.0244      561.
  O2(aq)           0.000251   0.000251      8.00
  SiO2(aq)        6.15e-005  6.15e-005      3.68
```

17) BASIN 3 CHEMISTRY AFTER ALKALINE DISCHARGE FROM BASIN 2, FLASH MIX RATIO=0.016

```
        Step #    16             Xi = 0.0160
          Temperature =  25.0 C    Pressure =  1.013 bars
          pH =  3.045              log fO2 =   -0.699
          Eh =   1.0385 volts      pe =  17.5557
          Ionic strength      =    0.026395
          Activity of water   =    1.000000
          Solvent mass        =    1.000000 kg
          Solution mass       =    1.002207 kg
          Solution density    =    1.014    g/cm3
          Chlorinity          =    0.000000 molal
          Dissolved solids    =        2202 mg/kg sol'n
          Elect. conductivity =     2568.29 uS/cm (or umho/cm)
          Hardness            =       35.32 mg/kg sol'n as CaCO3
            carbonate         =        0.00 mg/kg sol'n as CaCO3
            non-carbonate     =       35.32 mg/kg sol'n as CaCO3
          Rock mass           =    0.000000 kg
          Carbonate alkalinity=        0.00 mg/kg sol'n as CaCO3
          Water type          =    Na-NO3
```

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			
Ca++	0.0003897	6.336e-006	0.0002539	
H+	8.472e-006	1.378e-007	1.388e-007	
H2O	54.62	0.8881	16.00	
NO3-	0.02470	0.0004016	0.02490	
Na+	0.02312	0.0003760	0.008644	
O2(g)	-- fixed fugacity buffer --			
SiO2(aq)	6.396e-005	1.040e-006	6.249e-005	

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
NO3-	0.02608	1613.	0.8507	-1.6540
Na+	0.02439	559.4	0.8568	-1.6800
H+	0.001022	1.028	0.8814	-3.0452
Ca++	0.0003169	12.67	0.5629	-3.7487
O2(aq)	0.0002506	8.003	1.0069	-3.5980
SiO2(aq)	6.156e-005	3.690	1.0069	-4.2078
CaNO3+	3.682e-005	3.750	0.8568	-4.5011
CO2(aq)	1.116e-005	0.4900	1.0000	-4.9524

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Quartz	-0.2085	Cristobalite	-0.7590
Tridymite	-0.3743	Amrph^silica	-1.4942
Chalcedony	-0.4797		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.2000	-0.699
Steam	0.03131	-1.504
CO2(g)	0.0003162	-3.500
N2(g)	1.102e-005	-4.958
H2(g)	6.282e-042	-41.202
CH4(g)	3.888e-146	-145.410

		In fluid		Sorbed		Kd
Original basis	total moles	moles	mg/kg	moles	mg/kg	L/kg
Ca++	0.000354	0.000354	14.1			
H+	0.00103	0.00103	1.04			
H2O	55.5	55.5	9.98e+005			
HCO3-	1.12e-005	1.12e-005	0.680			
NO3-	0.0261	0.0261	1.62e+003			
Na+	0.0244	0.0244	559.			
O2(aq)	0.000251	0.000251	8.00			
SiO2(aq)	6.16e-005	6.16e-005	3.69			

APPENDIX C. GWB OUTPUT FILES: 1 MONTH DISCHARGE DURATION

1) STARTING SOLUTION CHEMISTRY FOR BASIN 1

```
          Temperature =  25.0 C    Pressure =  1.013 bars
          pH =  3.044              log fO2 =   -0.699
          Eh =   1.0386 volts      pe =  17.5566
          Ionic strength      =    0.026462
          Activity of water   =    1.000000
          Solvent mass        =    1.000005 kg
          Solution mass       =    1.002218 kg
          Solution density    =    1.014    g/cm3
          Chlorinity          =    0.000000 molal
          Dissolved solids    =        2208 mg/kg sol'n
          Elect. conductivity =     2573.82 uS/cm (or umho/cm)
          Hardness            =       35.52 mg/kg sol'n as CaCO3
            carbonate         =        0.00 mg/kg sol'n as CaCO3
            non-carbonate     =       35.52 mg/kg sol'n as CaCO3
          Rock mass           =    0.000000 kg
          Carbonate alkalinity=        0.00 mg/kg sol'n as CaCO3
          Water type          =    Na-NO3
```

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			
Ca++	5.315e-005	5.315e-005	0.002130	
CaCO3	0.0003025	0.0003025	0.03028	
H+	4.418e-013	4.418e-013	4.453e-013	
H2O	27.75	27.75	500.0	
NO3-	0.0007169	0.0007169	0.04445	
Na+	0.008228	0.008228	0.1892	
O2(g)	-- fixed fugacity buffer --			
SiO2(aq)	4.521e-005	4.521e-005	0.002716	

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
NO3-	0.02614	1617.	0.8505	-1.6529
Na+	0.02444	560.7	0.8567	-1.6790
H+	0.001024	1.030	0.8813	-3.0444
Ca++	0.0003186	12.74	0.5625	-3.7466
O2(aq)	0.0002506	8.003	1.0069	-3.5980
SiO2(aq)	6.167e-005	3.697	1.0069	-4.2070
CaNO3+	3.709e-005	3.778	0.8567	-4.4980
CO2(aq)	1.116e-005	0.4900	1.0000	-4.9524

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Quartz	-0.2077	Cristobalite	-0.7582
Tridymite	-0.3735	Amrph^silica	-1.4934
Chalcedony	-0.4789		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.2000	-0.699
Steam	0.03131	-1.504
CO2(g)	0.0003162	-3.500
N2(g)	1.111e-005	-4.954
H2(g)	6.282e-042	-41.202
CH4(g)	3.888e-146	-145.410

		In fluid		Sorbed		Kd
Original basis	total moles	moles	mg/kg	moles	mg/kg	L/kg
Ca++	0.000356	0.000356	14.2			
H+	0.00104	0.00104	1.04			
H2O	55.5	55.5	9.98e+005			
HCO3-	1.12e-005	1.12e-005	0.680			
NO3-	0.0262	0.0262	1.62e+003			
Na+	0.0244	0.0244	561.			
O2(aq)	0.000251	0.000251	8.00			
SiO2(aq)	6.17e-005	6.17e-005	3.70			

2) BASIN 1 CHEMISTRY AFTER ACIDIC WASTE STREAM, FLASH MIX RATIO=0.811

Step # 811 Xi = 0.8110
Temperature = 25.0 C Pressure = 1.013 bars
pH = 2.609 log fO2 = -0.699
Eh = 1.0643 volts pe = 17.9922
Ionic strength = 0.033895
Activity of water = 1.000000
Solvent mass = 1.000000 kg
Solution mass = 1.002825 kg
Solution density = 1.014 g/cm3
Chlorinity = 0.000000 molal
Dissolved solids = 2817 mg/kg sol'n
Elect. conductivity = 3548.13 uS/cm (or umho/cm)
Hardness = 6.72 mg/kg sol'n as CaCO3
carbonate = 0.00 mg/kg sol'n as CaCO3
non-carbonate = 6.72 mg/kg sol'n as CaCO3
Rock mass = 0.000000 kg
Carbonate alkalinity= 0.00 mg/kg sol'n as CaCO3
Water type = Na-NO3

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			
H+	0.0006124	0.002628	0.002648	
H2O	10.49	45.02	811.0	
NO3-	0.006747	0.02895	1.795	
Na+	0.006124	0.02628	0.6041	
O2(g)	-- fixed fugacity buffer --			
SiO2(aq)	6.218e-006	2.668e-005	0.001603	

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
NO3-	0.03384	2092.	0.8357	-1.5486
Na+	0.03089	708.1	0.8431	-1.5843
H+	0.002822	2.836	0.8723	-2.6088
O2(aq)	0.0002502	7.982	1.0088	-3.5980
Ca++	5.890e-005	2.354	0.5324	-4.5037
SiO2(aq)	3.834e-005	2.297	1.0088	-4.4125
CO2(aq)	1.116e-005	0.4897	1.0000	-4.9524
CaNO3+	8.384e-006	0.8534	0.8431	-5.1507
N2(aq)	8.727e-008	0.002438	1.0000	-7.0591

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Quartz	-0.4132	Cristobalite	-0.9637
Tridymite	-0.5790	Amrph^silica	-1.6989
Chalcedony	-0.6844		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.2000	-0.699
Steam	0.03131	-1.504
CO2(g)	0.0003162	-3.500
N2(g)	0.0001336	-3.874
H2(g)	6.282e-042	-41.202
CH4(g)	3.888e-146	-145.410

		In fluid		Sorbed		Kd
Original basis	total moles	moles	mg/kg	moles	mg/kg	L/kg
Ca++	6.73e-005	6.73e-005	2.69			
H+	0.00283	0.00283	2.85			
H2O	55.5	55.5	9.97e+005			
HCO3-	1.12e-005	1.12e-005	0.679			
NO3-	0.0338	0.0338	2.09e+003			
Na+	0.0309	0.0309	708.			
O2(aq)	0.000250	0.000250	7.98			
SiO2(aq)	3.83e-005	3.83e-005	2.30			

3) BASIN 1 CHEMISTRY AFTER ALKALINE WASTE STREAM, FLASH MIX RATIO=0.964

Step # 964 Xi = 0.9640
Temperature = 25.0 C Pressure = 1.013 bars
pH = 8.237 log fO2 = -0.699
Eh = 0.7314 volts pe = 12.3642
Ionic strength = 0.018820
Activity of water = 1.000000
Solvent mass = 0.999992 kg
Solution mass = 1.001555 kg
Solution density = 1.014 g/cm3
Chlorinity = 0.000000 molal
Dissolved solids = 1560 mg/kg sol'n

```
        Elect. conductivity =     1684.93 uS/cm (or umho/cm)
        Hardness            =       65.69 mg/kg sol'n as CaCO3
          carbonate         =       49.67 mg/kg sol'n as CaCO3
          non-carbonate     =       16.02 mg/kg sol'n as CaCO3
        Rock mass           =    0.000003 kg
        Carbonate alkalinity=       49.67 mg/kg sol'n as CaCO3
        Water type          =    Na-NO3
```

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			
Ca++	3.827e-006	0.0001025	0.004107	
CaCO3	2.178e-005	0.0005833	0.05838	
H+	3.181e-014	8.518e-013	8.586e-013	
H2O	1.998	53.51	964.0	
NO3-	5.162e-005	0.001382	0.08570	
Na+	0.0005924	0.01586	0.3647	
O2(g)	-- fixed fugacity buffer --			
SiO2(aq)	3.255e-006	8.716e-005	0.005237	

Minerals in system	moles	log moles	grams	volume (cm3)
Calcite	3.080e-005	-4.512	0.003082	0.001137
(total)			0.003082	0.001137

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
NO3-	0.01724	1067.	0.8694	-1.8243
Na+	0.01696	389.3	0.8741	-1.8290
HCO3-	0.0009456	57.61	0.8764	-3.0816
Ca++	0.0005984	23.95	0.6037	-3.4422
O2(aq)	0.0002511	8.024	1.0049	-3.5980
SiO2(aq)	8.541e-005	5.124	1.0049	-4.0664
CaNO3+	4.938e-005	5.033	0.8741	-4.3649
NaHCO3	1.653e-005	1.387	1.0000	-4.7816
CO2(aq)	1.116e-005	0.4903	1.0000	-4.9524
CO3--	1.104e-005	0.6613	0.5867	-5.1887
CaHCO3+	5.676e-006	0.5729	0.8794	-5.3018
CaCO3	3.846e-006	0.3843	1.0000	-5.4150
H3SiO4-	2.631e-006	0.2498	0.8741	-5.6384
OH-	2.040e-006	0.03464	0.8718	-5.7500
NaH3SiO4	4.807e-007	0.05668	1.0000	-6.3181
NaCO3-	3.507e-007	0.02907	0.8741	-6.5134
CaH3SiO4+	1.777e-008	0.002398	0.8741	-7.8089
NaOH	1.654e-008	0.0006607	1.0000	-7.7813
CaOH+	1.460e-008	0.0008321	0.8741	-7.8941

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Calcite	0.0000 sat	Chalcedony	-0.3383
Quartz	-0.0671	Cristobalite	-0.6176
Aragonite	-0.1649	Monohydrocalcite	-0.9939
Tridymite	-0.2329	Amrph^silica	-1.3528

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.2000	-0.699
Steam	0.03131	-1.504
CO2(g)	0.0003162	-3.500
N2(g)	2.081e-016	-15.682
H2(g)	6.282e-042	-41.202
CH4(g)	3.888e-146	-145.410

		In fluid		Sorbed		Kd
Original basis	total moles	moles	mg/kg	moles	mg/kg	L/kg
Ca++	0.000688	0.000657	26.3			
H+	-4.01e-005	-9.27e-006	-0.00933			
H2O	55.5	55.5	9.98e+005			
HCO3-	0.00102	0.000994	60.6			
NO3-	0.0173	0.0173	1.07e+003			
Na+	0.0170	0.0170	390.			
O2(aq)	0.000251	0.000251	8.02			
SiO2(aq)	8.85e-005	8.85e-005	5.31			

4) BASIN 1 CHEMISTRY AFTER ACIDIC WASTE STREAM, FLASH MIX RATIO=0.964

Step #	964	Xi	= 0.9640
Temperature =	25.0 C	Pressure =	1.013 bars
pH =	2.581	log fO2 =	-0.699
Eh =	1.0660 volts	pe =	18.0197
Ionic strength	=	0.035029	
Activity of water	=	1.000000	
Solvent mass	=	1.000001 kg	
Solution mass	=	1.002919 kg	
Solution density	=	1.014 g/cm3	
Chlorinity	=	0.000000 molal	
Dissolved solids	=	2909 mg/kg sol'n	
Elect. conductivity	=	3672.09 uS/cm (or umho/cm)	
Hardness	=	6.26 mg/kg sol'n as CaCO3	
carbonate	=	0.00 mg/kg sol'n as CaCO3	
non-carbonate	=	6.26 mg/kg sol'n as CaCO3	
Rock mass	=	0.000000 kg	
Carbonate alkalinity	=	0.00 mg/kg sol'n as CaCO3	
Water type	=	Na-NO3	

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			
Calcite	1.109e-006	2.969e-005	0.002972	0.001097
H+	0.0001166	0.003123	0.003148	
H2O	1.998	53.51	964.0	
NO3-	0.001285	0.03441	2.134	
Na+	0.001166	0.03123	0.7181	
O2(g)	-- fixed fugacity buffer --			
SiO2(aq)	1.184e-006	3.172e-005	0.001906	

```
 No minerals in system.

 Aqueous species       molality    mg/kg sol'n    act. coef.     log act.
-------------------------------------------------------------------------
  NO3-                  0.03497         2162.      0.8336       -1.5353
  Na+                   0.03185         730.0      0.8413       -1.5720
  H+                   0.003011         3.026      0.8711       -2.5812
  O2(aq)              0.0002501         7.979      1.0091       -3.5980
  Ca++                5.476e-005         2.188      0.5283       -4.5387
  SiO2(aq)            3.490e-005         2.091      1.0091       -4.4532
  CO2(aq)             1.116e-005        0.4896      1.0000       -4.9524
  CaNO3+              7.993e-006        0.8136      0.8413       -5.1723
  N2(aq)              1.053e-007      0.002943      1.0000       -6.9774
   (only species > 1e-8 molal listed)

 Mineral saturation states
                    log Q/K                              log Q/K
-------------------------------------------------------------------
  Quartz            -0.4539        Cristobalite       -1.0044
  Tridymite         -0.6197        Amrph^silica       -1.7396
  Chalcedony        -0.7251
   (only minerals with log Q/K > -3 listed)

 Gases                 fugacity      log fug.
-----------------------------------------------
  O2(g)                   0.2000       -0.699
  Steam                  0.03131       -1.504
  CO2(g)               0.0003162       -3.500
  N2(g)                0.0001612       -3.793
  H2(g)                6.282e-042     -41.202
  CH4(g)               3.888e-146    -145.410

                                  In fluid              Sorbed             Kd
 Original basis total moles   moles     mg/kg      moles     mg/kg      L/kg
-------------------------------------------------------------------------------
---
  Ca++           6.27e-005  6.27e-005      2.51
  H+               0.00302    0.00302      3.04
  H2O                 55.5       55.5 9.97e+005
  HCO3-          1.12e-005  1.12e-005     0.679
  NO3-              0.0350     0.0350 2.16e+003
  Na+               0.0318     0.0318      730.
  O2(aq)          0.000250   0.000250      7.97
  SiO2(aq)       3.49e-005  3.49e-005      2.09
```

5) BASIN 1 CHEMISTRY AFTER ALKALINE WASTE STREAM, FLASH MIX RATIO=0.964

```
         Step #   964             Xi = 0.9640
          Temperature =  25.0 C    Pressure =  1.013 bars
          pH =  8.236              log fO2 =   -0.699
          Eh =   0.7314 volts      pe =  12.3649
          Ionic strength      =    0.018859
          Activity of water   =    1.000000
          Solvent mass        =    0.999992 kg
          Solution mass       =    1.001558 kg
          Solution density    =    1.014    g/cm3
```

```
        Chlorinity          =    0.000000 molal
        Dissolved solids    =        1563 mg/kg sol'n
        Elect. conductivity =     1688.07 uS/cm (or umho/cm)
        Hardness            =       65.95 mg/kg sol'n as CaCO3
          carbonate         =       49.59 mg/kg sol'n as CaCO3
          non-carbonate     =       16.35 mg/kg sol'n as CaCO3
        Rock mass           =    0.000003 kg
        Carbonate alkalinity=       49.59 mg/kg sol'n as CaCO3
        Water type          =    Na-NO3
```

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			
Ca++	3.827e-006	0.0001025	0.004107	
CaCO3	2.178e-005	0.0005833	0.05838	
H+	3.181e-014	8.518e-013	8.586e-013	
H2O	1.998	53.51	964.0	
NO3-	5.162e-005	0.001382	0.08570	
Na+	0.0005924	0.01586	0.3647	
O2(g)	-- fixed fugacity buffer --			
SiO2(aq)	3.255e-006	8.716e-005	0.005237	

Minerals in system	moles	log moles	grams	volume (cm3)
Calcite	2.808e-005	-4.552	0.002811	0.001037
(total)			0.002811	0.001037

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
NO3-	0.01728	1070.	0.8693	-1.8234
Na+	0.01699	390.0	0.8740	-1.8283
HCO3-	0.0009441	57.52	0.8763	-3.0823
Ca++	0.0006007	24.04	0.6034	-3.4407
O2(aq)	0.0002511	8.023	1.0049	-3.5980
SiO2(aq)	8.530e-005	5.117	1.0049	-4.0669
CaNO3+	4.966e-005	5.061	0.8740	-4.3625
NaHCO3	1.654e-005	1.387	1.0000	-4.7816
CO2(aq)	1.116e-005	0.4903	1.0000	-4.9524
CO3--	1.101e-005	0.6594	0.5865	-5.1902
CaHCO3+	5.686e-006	0.5739	0.8793	-5.3011
CaCO3	3.846e-006	0.3843	1.0000	-5.4150
H3SiO4-	2.623e-006	0.2491	0.8740	-5.6397
OH-	2.037e-006	0.03458	0.8717	-5.7507
NaH3SiO4	4.802e-007	0.05662	1.0000	-6.3186
NaCO3-	3.502e-007	0.02902	0.8740	-6.5141
CaH3SiO4+	1.777e-008	0.002399	0.8740	-7.8087
NaOH	1.655e-008	0.0006608	1.0000	-7.7813
CaOH+	1.463e-008	0.0008336	0.8740	-7.8934

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Calcite	0.0000 sat	Chalcedony	-0.3388
Quartz	-0.0676	Cristobalite	-0.6181

```
   Aragonite          -0.1649        Monohydrocalcite  -0.9939
   Tridymite          -0.2334        Amrph^silica      -1.3533
    (only minerals with log Q/K > -3 listed)

  Gases                 fugacity      log fug.
 ------------------------------------------------
   O2(g)                    0.2000      -0.699
   Steam                  0.03131      -1.504
   CO2(g)                0.0003162      -3.500
   N2(g)                2.097e-016     -15.678
   H2(g)                6.282e-042     -41.202
   CH4(g)               3.888e-146    -145.410

                                  In fluid              Sorbed            Kd
  Original basis total moles   moles     mg/kg      moles     mg/kg      L/kg
 ---------------------------------------------------------------------------
---
   Ca++             0.000688   0.000660      26.4
   H+             -3.73e-005 -9.23e-006  -0.00929
   H2O                 55.5       55.5 9.98e+005
   HCO3-            0.00102   0.000993      60.5
   NO3-              0.0173     0.0173 1.07e+003
   Na+               0.0170     0.0170      390.
   O2(aq)          0.000251   0.000251      8.02
   SiO2(aq)       8.84e-005  8.84e-005      5.30
```

6) BASIN 1 CHEMISTRY AFTER ACIDIC WASTE STREAM, FLASH MIX RATIO=0.964

```
        Step #   964             Xi = 0.9640
          Temperature =  25.0 C    Pressure =  1.013 bars
          pH =  2.580              log fO2 =   -0.699
          Eh =   1.0660 volts      pe =  18.0208
          Ionic strength      =    0.035026
          Activity of water   =    1.000000
          Solvent mass        =    1.000001 kg
          Solution mass       =    1.002918 kg
          Solution density    =    1.014    g/cm3
          Chlorinity          =    0.000000 molal
          Dissolved solids    =        2909 mg/kg sol'n
          Elect. conductivity =     3673.65 uS/cm (or umho/cm)
          Hardness            =        5.92 mg/kg sol'n as CaCO3
            carbonate         =        0.00 mg/kg sol'n as CaCO3
            non-carbonate     =        5.92 mg/kg sol'n as CaCO3
          Rock mass           =    0.000000 kg
          Carbonate alkalinity=        0.00 mg/kg sol'n as CaCO3
          Water type          =    Na-NO3

                           moles        moles         grams          cm3
  Reactants              remaining     reacted       reacted       reacted
 ---------------------------------------------------------------------------
   CO2(g)              -- fixed fugacity buffer --
   Calcite             1.011e-006    2.707e-005      0.002709     0.0009998
   H+                   0.0001166      0.003123      0.003148
   H2O                      1.998         53.51         964.0
   NO3-                  0.001285       0.03441         2.134
   Na+                   0.001166       0.03123        0.7181
   O2(g)               -- fixed fugacity buffer --
```

```
  SiO2(aq)            1.184e-006    3.172e-005      0.001906

 No minerals in system.

 Aqueous species       molality    mg/kg sol'n    act. coef.     log act.
-------------------------------------------------------------------------
  NO3-                  0.03497         2162.      0.8336       -1.5353
  Na+                   0.03185         730.0      0.8413       -1.5720
  H+                   0.003018         3.033      0.8711       -2.5802
  O2(aq)              0.0002501         7.979      1.0091       -3.5980
  Ca++                5.173e-005         2.067      0.5283       -4.5634
  SiO2(aq)            3.490e-005         2.091      1.0091       -4.4533
  CO2(aq)             1.116e-005        0.4896      1.0000       -4.9524
  CaNO3+              7.551e-006        0.7686      0.8413       -5.1970
  N2(aq)              1.058e-007      0.002956      1.0000       -6.9753
   (only species > 1e-8 molal listed)

 Mineral saturation states
                    log Q/K                            log Q/K
-----------------------------------------------------------------
  Quartz            -0.4540        Cristobalite      -1.0045
  Tridymite         -0.6198        Amrph^silica      -1.7397
  Chalcedony        -0.7252
   (only minerals with log Q/K > -3 listed)

 Gases                fugacity      log fug.
------------------------------------------------
  O2(g)                 0.2000        -0.699
  Steam                0.03131        -1.504
  CO2(g)              0.0003162        -3.500
  N2(g)               0.0001620        -3.791
  H2(g)               6.282e-042      -41.202
  CH4(g)              3.888e-146     -145.410

                                  In fluid              Sorbed             Kd
 Original basis total moles   moles     mg/kg      moles     mg/kg       L/kg
-------------------------------------------------------------------------------
---
  Ca++           5.93e-005  5.93e-005      2.37
  H+               0.00303    0.00303      3.04
  H2O                 55.5       55.5 9.97e+005
  HCO3-          1.12e-005  1.12e-005     0.679
  NO3-              0.0350     0.0350 2.16e+003
  Na+               0.0318     0.0318      730.
  O2(aq)          0.000250   0.000250      7.97
  SiO2(aq)       3.49e-005  3.49e-005      2.09
```

7) STARTING SOLUTION CHEMISTRY FOR BASIN 2

```
          Temperature =  25.0 C    Pressure =  1.013 bars
          pH =  3.044              log fO2 =   -0.699
          Eh =   1.0386 volts      pe =  17.5566
          Ionic strength      =    0.026462
          Activity of water   =    1.000000
          Solvent mass        =    1.000005 kg
          Solution mass       =    1.002218 kg
          Solution density    =    1.014    g/cm3
```

```
        Chlorinity          =    0.000000 molal
        Dissolved solids    =        2208 mg/kg sol'n
        Elect. conductivity =     2573.82 uS/cm (or umho/cm)
        Hardness            =       35.52 mg/kg sol'n as CaCO3
          carbonate         =        0.00 mg/kg sol'n as CaCO3
          non-carbonate     =       35.52 mg/kg sol'n as CaCO3
        Rock mass           =    0.000000 kg
        Carbonate alkalinity=        0.00 mg/kg sol'n as CaCO3
        Water type          =    Na-NO3
```

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			
Ca++	5.315e-005	5.315e-005	0.002130	
CaCO3	0.0003025	0.0003025	0.03028	
H+	4.418e-013	4.418e-013	4.453e-013	
H2O	27.75	27.75	500.0	
NO3-	0.0007169	0.0007169	0.04445	
Na+	0.008228	0.008228	0.1892	
O2(g)	-- fixed fugacity buffer --			
SiO2(aq)	4.521e-005	4.521e-005	0.002716	

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
NO3-	0.02614	1617.	0.8505	-1.6529
Na+	0.02444	560.7	0.8567	-1.6790
H+	0.001024	1.030	0.8813	-3.0444
Ca++	0.0003186	12.74	0.5625	-3.7466
O2(aq)	0.0002506	8.003	1.0069	-3.5980
SiO2(aq)	6.167e-005	3.697	1.0069	-4.2070
CaNO3+	3.709e-005	3.778	0.8567	-4.4980
CO2(aq)	1.116e-005	0.4900	1.0000	-4.9524

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Quartz	-0.2077	Cristobalite	-0.7582
Tridymite	-0.3735	Amrph^silica	-1.4934
Chalcedony	-0.4789		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.2000	-0.699
Steam	0.03131	-1.504
CO2(g)	0.0003162	-3.500
N2(g)	1.111e-005	-4.954
H2(g)	6.282e-042	-41.202
CH4(g)	3.888e-146	-145.410

		In fluid		Sorbed		Kd
Original basis	total moles	moles	mg/kg	moles	mg/kg	L/kg

```
 ------------------------------------------------------------------------
---
   Ca++            0.000356   0.000356      14.2
   H+               0.00104    0.00104      1.04
   H2O                 55.5       55.5 9.98e+005
   HCO3-           1.12e-005  1.12e-005     0.680
   NO3-               0.0262     0.0262 1.62e+003
   Na+                0.0244     0.0244      561.
   O2(aq)           0.000251   0.000251      8.00
   SiO2(aq)        6.17e-005  6.17e-005      3.70
```

8) BASIN 2 CHEMISTRY AFTER ACIDIC DISCHARGE FROM BASIN 1, FLASH MIX RATIO=0.675

```
       Step #   675             Xi = 0.6750
          Temperature =  25.0 C    Pressure =  1.013 bars
          pH =  2.901              log fO2 =   -0.699
          Eh =   1.0470 volts      pe =  17.6997
          Ionic strength      =    0.028160
          Activity of water   =    1.000000
          Solvent mass        =    1.000000 kg
          Solution mass       =    1.002352 kg
          Solution density    =    1.014    g/cm3
          Chlorinity          =    0.000000 molal
          Dissolved solids    =        2346 mg/kg sol'n
          Elect. conductivity =     2797.91 uS/cm (or umho/cm)
          Hardness            =       30.43 mg/kg sol'n as CaCO3
            carbonate         =        0.00 mg/kg sol'n as CaCO3
            non-carbonate     =       30.43 mg/kg sol'n as CaCO3
          Rock mass           =    0.000000 kg
          Carbonate alkalinity=        0.00 mg/kg sol'n as CaCO3
          Water type          =    Na-NO3

                          moles        moles         grams          cm3
 Reactants              remaining     reacted       reacted       reacted
 ------------------------------------------------------------------------
  CO2(g)              -- fixed fugacity buffer --
  Ca++                9.100e-005     0.0001890      0.007575
  H+                   0.0005265      0.001093      0.001102
  H2O                      18.04         37.47         675.0
  NO3-                  0.009360       0.01944         1.205
  Na+                   0.008645       0.01796        0.4128
  O2(g)               -- fixed fugacity buffer --
  SiO2(aq)            1.745e-005    3.625e-005      0.002178

 No minerals in system.

 Aqueous species       molality    mg/kg sol'n    act. coef.     log act.
 ------------------------------------------------------------------------
  NO3-                  0.02789         1725.      0.8469       -1.6267
  Na+                   0.02589         593.7      0.8534       -1.6558
  H+                   0.001428         1.436      0.8791       -2.9013
  Ca++                0.0002715         10.85      0.5550       -3.8220
  O2(aq)              0.0002505         7.998      1.0073       -3.5980
  SiO2(aq)            5.630e-005         3.375      1.0073       -4.2463
  CaNO3+              3.324e-005         3.386      0.8534       -4.5472
  CO2(aq)             1.116e-005        0.4899      1.0000       -4.9524
```

```
  N2(aq)              1.583e-008     0.0004425      1.0000       -7.8004
    (only species > 1e-8 molal listed)

 Mineral saturation states
                    log Q/K                            log Q/K
-------------------------------------------------------------------
  Quartz            -0.2470        Cristobalite      -0.7975
  Tridymite         -0.4128        Amrph^silica      -1.5327
  Chalcedony        -0.5182
    (only minerals with log Q/K > -3 listed)

 Gases                fugacity      log fug.
-----------------------------------------------
  O2(g)                   0.2000      -0.699
  Steam                  0.03131      -1.504
  CO2(g)               0.0003162      -3.500
  N2(g)                2.423e-005     -4.616
  H2(g)                6.282e-042    -41.202
  CH4(g)               3.888e-146    -145.410

                                  In fluid              Sorbed            Kd
 Original basis total moles   moles     mg/kg      moles     mg/kg      L/kg
-------------------------------------------------------------------------------
---
  Ca++            0.000305   0.000305      12.2
  H+               0.00144    0.00144      1.45
  H2O                 55.5       55.5 9.98e+005
  HCO3-           1.12e-005  1.12e-005     0.680
  NO3-               0.0279     0.0279 1.73e+003
  Na+                0.0259     0.0259      594.
  O2(aq)           0.000250   0.000250      8.00
  SiO2(aq)        5.63e-005  5.63e-005      3.37
```

9) BASIN 2 CHEMISTRY AFTER ALKALINE DISCHARGE FROM BASIN 1, FLASH MIX RATIO=0.718

```
  Step #   718             Xi = 0.7180
        Temperature =  25.0 C    Pressure =  1.013 bars
        pH =  3.443              log fO2 =   -0.699
        Eh =   1.0150 volts      pe =  17.1582
        Ionic strength      =    0.022942
        Activity of water   =    1.000000
        Solvent mass        =    1.000000 kg
        Solution mass       =    1.001915 kg
        Solution density    =    1.014    g/cm3
        Chlorinity          =    0.000000 molal
        Dissolved solids    =        1912 mg/kg sol'n
        Elect. conductivity =     2145.82 uS/cm (or umho/cm)
        Hardness            =       51.34 mg/kg sol'n as CaCO3
          carbonate         =        0.00 mg/kg sol'n as CaCO3
          non-carbonate     =       51.34 mg/kg sol'n as CaCO3
        Rock mass           =    0.000000 kg
        Carbonate alkalinity=        0.00 mg/kg sol'n as CaCO3
        Water type          =    Na-NO3

                          moles        moles         grams          cm3
 Reactants              remaining     reacted       reacted       reacted
```

CO2(g)	-- fixed fugacity buffer --		
Ca++	0.0001681	0.0004279	0.01715
H+	1.585e-006	4.035e-006	4.067e-006
H2O	15.65	39.86	718.0
NO3-	0.005612	0.01429	0.8859
Na+	0.005414	0.01379	0.3169
O2(g)	-- fixed fugacity buffer --		
SiO2(aq)	2.270e-005	5.780e-005	0.003473

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
NO3-	0.02248	1391.	0.8587	-1.7145
Na+	0.02109	483.9	0.8642	-1.7393
Ca++	0.0004658	18.64	0.5799	-3.5684
H+	0.0004070	0.4094	0.8865	-3.4428
O2(aq)	0.0002509	8.012	1.0060	-3.5980
SiO2(aq)	7.368e-005	4.418	1.0060	-4.1301
CaNO3+	4.810e-005	4.900	0.8642	-4.3813
CO2(aq)	1.116e-005	0.4901	1.0000	-4.9524
HCO3-	1.536e-008	0.0009356	0.8668	-7.8756

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Quartz	-0.1308	Cristobalite	-0.6813
Tridymite	-0.2966	Amrph^silica	-1.4165
Chalcedony	-0.4020		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.2000	-0.699
Steam	0.03131	-1.504
CO2(g)	0.0003162	-3.500
N2(g)	1.337e-006	-5.874
H2(g)	6.282e-042	-41.202
CH4(g)	3.888e-146	-145.410

		In fluid		Sorbed		Kd
Original basis	total moles	moles	mg/kg	moles	mg/kg	L/kg
Ca++	0.000514	0.000514	20.6			
H+	0.000418	0.000418	0.421			
H2O	55.5	55.5	9.98e+005			
HCO3-	1.12e-005	1.12e-005	0.681			
NO3-	0.0225	0.0225	1.39e+003			
Na+	0.0211	0.0211	484.			
O2(aq)	0.000251	0.000251	8.01			
SiO2(aq)	7.37e-005	7.37e-005	4.42			

10) BASIN 2 CHEMISTRY AFTER ACIDIC DISCHARGE FROM BASIN 1, FLASH MIX RATIO=0.894

```
     Step #   894             Xi = 0.8940
          Temperature =  25.0 C    Pressure =  1.013 bars
          pH =  2.883              log fO2 =   -0.699
          Eh =   1.0481 volts      pe =  17.7184
          Ionic strength      =    0.028356
          Activity of water   =    1.000000
          Solvent mass        =    1.000000 kg
          Solution mass       =    1.002367 kg
          Solution density    =    1.014    g/cm3
          Chlorinity          =    0.000000 molal
          Dissolved solids    =        2362 mg/kg sol'n
          Elect. conductivity =     2826.86 uS/cm (or umho/cm)
          Hardness            =       30.44 mg/kg sol'n as CaCO3
            carbonate         =        0.00 mg/kg sol'n as CaCO3
            non-carbonate     =       30.44 mg/kg sol'n as CaCO3
          Rock mass           =    0.000000 kg
          Carbonate alkalinity=        0.00 mg/kg sol'n as CaCO3
          Water type          =    Na-NO3
```

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			
Ca++	2.968e-005	0.0002503	0.01003	
H+	0.0001717	0.001448	0.001460	
H2O	5.884	49.62	894.0	
NO3-	0.003053	0.02575	1.596	
Na+	0.002820	0.02378	0.5467	
O2(g)	-- fixed fugacity buffer --			
SiO2(aq)	5.692e-006	4.801e-005	0.002885	

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
NO3-	0.02808	1737.	0.8465	-1.6239
Na+	0.02602	596.7	0.8530	-1.6538
H+	0.001491	1.500	0.8788	-2.8825
Ca++	0.0002714	10.85	0.5541	-3.8228
O2(aq)	0.0002505	7.997	1.0074	-3.5980
SiO2(aq)	5.582e-005	3.346	1.0074	-4.2500
CaNO3+	3.341e-005	3.403	0.8530	-4.5451
CO2(aq)	1.116e-005	0.4899	1.0000	-4.9524
N2(aq)	1.749e-008	0.0004888	1.0000	-7.7572

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Quartz	-0.2507	Cristobalite	-0.8012
Tridymite	-0.4165	Amrph^silica	-1.5364
Chalcedony	-0.5219		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.2000	-0.699
Steam	0.03131	-1.504
CO2(g)	0.0003162	-3.500
N2(g)	2.677e-005	-4.572
H2(g)	6.282e-042	-41.202
CH4(g)	3.888e-146	-145.410

		In fluid		Sorbed		Kd
Original basis	total moles	moles	mg/kg	moles	mg/kg	L/kg
Ca++	0.000305	0.000305	12.2			
H+	0.00150	0.00150	1.51			
H2O	55.5	55.5	9.98e+005			
HCO3-	1.12e-005	1.12e-005	0.680			
NO3-	0.0281	0.0281	1.74e+003			
Na+	0.0260	0.0260	597.			
O2(aq)	0.000250	0.000250	8.00			
SiO2(aq)	5.58e-005	5.58e-005	3.35			

11) BASIN 2 CHEMISTRY AFTER ALKALINE DISCHARGE FROM BASIN 1, FLASH MIX RATIO=0.718

Step # 718 Xi = 0.7180
Temperature = 25.0 C Pressure = 1.013 bars
pH = 3.425 log fO2 = -0.699
Eh = 1.0160 volts pe = 17.1758
Ionic strength = 0.022987
Activity of water = 1.000000
Solvent mass = 1.000000 kg
Solution mass = 1.001919 kg
Solution density = 1.014 g/cm3
Chlorinity = 0.000000 molal
Dissolved solids = 1915 mg/kg sol'n
Elect. conductivity = 2153.25 uS/cm (or umho/cm)
Hardness = 51.34 mg/kg sol'n as CaCO3
carbonate = 0.00 mg/kg sol'n as CaCO3
non-carbonate = 51.34 mg/kg sol'n as CaCO3
Rock mass = 0.000000 kg
Carbonate alkalinity= 0.00 mg/kg sol'n as CaCO3
Water type = Na-NO3

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			
Ca++	0.0001681	0.0004279	0.01715	
H+	1.585e-006	4.035e-006	4.067e-006	
H2O	15.65	39.86	718.0	
NO3-	0.005612	0.01429	0.8859	
Na+	0.005414	0.01379	0.3169	
O2(g)	-- fixed fugacity buffer --			
SiO2(aq)	2.270e-005	5.780e-005	0.003473	

```
 No minerals in system.

 Aqueous species       molality    mg/kg sol'n    act. coef.     log act.
-------------------------------------------------------------------------
  NO3-                  0.02252         1394.      0.8586       -1.7136
  Na+                   0.02112         484.6      0.8641       -1.7388
  Ca++                 0.0004658         18.63      0.5796       -3.5687
  H+                   0.0004239        0.4264      0.8864       -3.4251
  O2(aq)               0.0002509         8.012      1.0060       -3.5980
  SiO2(aq)            7.353e-005         4.410      1.0060       -4.1309
  CaNO3+              4.816e-005         4.907      0.8641       -4.3807
  CO2(aq)             1.116e-005        0.4901      1.0000       -4.9524
  HCO3-               1.475e-008     0.0008984      0.8667       -7.8933
   (only species > 1e-8 molal listed)

 Mineral saturation states
                    log Q/K                              log Q/K
-------------------------------------------------------------------
  Quartz            -0.1316        Cristobalite       -0.6821
  Tridymite         -0.2974        Amrph^silica       -1.4173
  Chalcedony        -0.4028
   (only minerals with log Q/K > -3 listed)

 Gases                 fugacity      log fug.
-----------------------------------------------
  O2(g)                   0.2000       -0.699
  Steam                  0.03131       -1.504
  CO2(g)                0.0003162       -3.500
  N2(g)                1.455e-006       -5.837
  H2(g)                6.282e-042      -41.202
  CH4(g)               3.888e-146     -145.410

                                  In fluid              Sorbed             Kd
 Original basis total moles   moles     mg/kg      moles     mg/kg       L/kg
-------------------------------------------------------------------------------
---
  Ca++            0.000514   0.000514      20.6
  H+              0.000435   0.000435     0.438
  H2O                 55.5       55.5 9.98e+005
  HCO3-          1.12e-005  1.12e-005     0.680
  NO3-              0.0226     0.0226 1.40e+003
  Na+               0.0211     0.0211      485.
  O2(aq)          0.000251   0.000251      8.01
  SiO2(aq)       7.35e-005  7.35e-005      4.41
```

12) BASIN 2 CHEMISTRY AFTER ALKALINE DISCHARGE FROM BASIN 1, FLASH MIX RATIO=0.894

```
     Step #   894             Xi = 0.8940
          Temperature =  25.0 C    Pressure =  1.013 bars
          pH =  2.882              log fO2 =   -0.699
          Eh =   1.0482 volts      pe =  17.7190
          Ionic strength      =    0.028358
          Activity of water   =    1.000000
          Solvent mass        =    1.000000 kg
          Solution mass       =    1.002367 kg
          Solution density    =    1.014    g/cm3
```

```
        Chlorinity          =    0.000000 molal
        Dissolved solids    =        2362 mg/kg sol'n
        Elect. conductivity =     2827.40 uS/cm (or umho/cm)
        Hardness            =       30.44 mg/kg sol'n as CaCO3
          carbonate         =        0.00 mg/kg sol'n as CaCO3
          non-carbonate     =       30.44 mg/kg sol'n as CaCO3
        Rock mass           =    0.000000 kg
        Carbonate alkalinity=        0.00 mg/kg sol'n as CaCO3
        Water type          =    Na-NO3
```

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			
Ca++	2.968e-005	0.0002503	0.01003	
H+	0.0001717	0.001448	0.001460	
H2O	5.884	49.62	894.0	
NO3-	0.003053	0.02575	1.596	
Na+	0.002820	0.02378	0.5467	
O2(g)	-- fixed fugacity buffer --			
SiO2(aq)	5.692e-006	4.801e-005	0.002885	

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
NO3-	0.02809	1737.	0.8465	-1.6239
Na+	0.02602	596.7	0.8530	-1.6538
H+	0.001493	1.501	0.8788	-2.8820
Ca++	0.0002714	10.85	0.5541	-3.8228
O2(aq)	0.0002505	7.997	1.0074	-3.5980
SiO2(aq)	5.580e-005	3.345	1.0074	-4.2502
CaNO3+	3.342e-005	3.403	0.8530	-4.5451
CO2(aq)	1.116e-005	0.4899	1.0000	-4.9524
N2(aq)	1.753e-008	0.0004900	1.0000	-7.7561

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Quartz	-0.2509	Cristobalite	-0.8014
Tridymite	-0.4167	Amrph^silica	-1.5366
Chalcedony	-0.5221		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.2000	-0.699
Steam	0.03131	-1.504
CO2(g)	0.0003162	-3.500
N2(g)	2.683e-005	-4.571
H2(g)	6.282e-042	-41.202
CH4(g)	3.888e-146	-145.410

		In fluid		Sorbed		Kd
Original basis	total moles	moles	mg/kg	moles	mg/kg	L/kg

```
 ------------------------------------------------------------------------------
---
   Ca++            0.000305   0.000305      12.2
   H+               0.00150    0.00150      1.51
   H2O                 55.5       55.5 9.98e+005
   HCO3-           1.12e-005  1.12e-005     0.680
   NO3-               0.0281     0.0281 1.74e+003
   Na+                0.0260     0.0260      597.
   O2(aq)          0.000250   0.000250      8.00
   SiO2(aq)        5.58e-005  5.58e-005      3.34
```

13) STARTING SOLUTION CHEMISTRY FOR BASIN 3

```
          Temperature =  25.0 C    Pressure =  1.013 bars
          pH =  3.044              log fO2 =   -0.699
          Eh =   1.0386 volts      pe =  17.5566
          Ionic strength      =    0.026462
          Activity of water   =    1.000000
          Solvent mass        =    1.000005 kg
          Solution mass       =    1.002218 kg
          Solution density    =    1.014    g/cm3
          Chlorinity          =    0.000000 molal
          Dissolved solids    =        2208 mg/kg sol'n
          Elect. conductivity =     2573.82 uS/cm (or umho/cm)
          Hardness            =       35.52 mg/kg sol'n as CaCO3
            carbonate         =        0.00 mg/kg sol'n as CaCO3
            non-carbonate     =       35.52 mg/kg sol'n as CaCO3
          Rock mass           =    0.000000 kg
          Carbonate alkalinity=        0.00 mg/kg sol'n as CaCO3
          Water type          =    Na-NO3
```

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			
Ca++	5.315e-005	5.315e-005	0.002130	
CaCO3	0.0003025	0.0003025	0.03028	
H+	4.418e-013	4.418e-013	4.453e-013	
H2O	27.75	27.75	500.0	
NO3-	0.0007169	0.0007169	0.04445	
Na+	0.008228	0.008228	0.1892	
O2(g)	-- fixed fugacity buffer --			
SiO2(aq)	4.521e-005	4.521e-005	0.002716	

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
NO3-	0.02614	1617.	0.8505	-1.6529
Na+	0.02444	560.7	0.8567	-1.6790
H+	0.001024	1.030	0.8813	-3.0444
Ca++	0.0003186	12.74	0.5625	-3.7466
O2(aq)	0.0002506	8.003	1.0069	-3.5980
SiO2(aq)	6.167e-005	3.697	1.0069	-4.2070
CaNO3+	3.709e-005	3.778	0.8567	-4.4980
CO2(aq)	1.116e-005	0.4900	1.0000	-4.9524

(only species > 1e-8 molal listed)

```
 Mineral saturation states
                    log Q/K                              log Q/K
-------------------------------------------------------------------
  Quartz            -0.2077       Cristobalite      -0.7582
  Tridymite         -0.3735       Amrph^silica      -1.4934
  Chalcedony        -0.4789
   (only minerals with log Q/K > -3 listed)

 Gases                fugacity      log fug.
-----------------------------------------------
  O2(g)                  0.2000       -0.699
  Steam                 0.03131       -1.504
  CO2(g)               0.0003162       -3.500
  N2(g)                1.111e-005       -4.954
  H2(g)                6.282e-042      -41.202
  CH4(g)               3.888e-146     -145.410

                                  In fluid              Sorbed            Kd
 Original basis total moles   moles     mg/kg      moles     mg/kg      L/kg
-------------------------------------------------------------------------------
--
   Ca++            0.000356   0.000356      14.2
   H+               0.00104    0.00104      1.04
   H2O                 55.5       55.5 9.98e+005
   HCO3-          1.12e-005  1.12e-005     0.680
   NO3-               0.0262     0.0262 1.62e+003
   Na+                0.0244     0.0244      561.
   O2(aq)           0.000251   0.000251      8.00
   SiO2(aq)        6.17e-005  6.17e-005      3.70
```

14) BASIN 3 CHEMISTRY AFTER ACIDIC DISCHARGE FROM BASIN 2, FLASH MIX RATIO=0.185

```
        Step #   185             Xi = 0.1850
          Temperature =  25.0 C    Pressure =  1.013 bars
          pH =  3.033              log fO2 =   -0.699
          Eh =   1.0392 volts      pe =  17.5678
          Ionic strength      =    0.026455
          Activity of water   =    1.000000
          Solvent mass        =    1.000000 kg
          Solution mass       =    1.002211 kg
          Solution density    =    1.014    g/cm3
          Chlorinity          =    0.000000 molal
          Dissolved solids    =        2206 mg/kg sol'n
          Elect. conductivity =     2578.91 uS/cm (or umho/cm)
          Hardness            =       35.90 mg/kg sol'n as CaCO3
            carbonate         =        0.00 mg/kg sol'n as CaCO3
            non-carbonate     =       35.90 mg/kg sol'n as CaCO3
          Rock mass           =    0.000000 kg
          Carbonate alkalinity=        0.00 mg/kg sol'n as CaCO3
          Water type          =    Na-NO3

                           moles        moles         grams          cm3
 Reactants               remaining     reacted       reacted       reacted
-------------------------------------------------------------------------------
  CO2(g)              -- fixed fugacity buffer --
```

```
  Ca++                 0.0003056    6.937e-005      0.002781
  H+                   0.0009372     0.0002128     0.0002144
  H2O                      45.24         10.27         185.0
  NO3-                   0.02143      0.004865        0.3017
  Na+                    0.01989      0.004514        0.1038
  O2(g)               -- fixed fugacity buffer --
  SiO2(aq)            5.029e-005    1.141e-005     0.0006858

 No minerals in system.

 Aqueous species       molality    mg/kg sol'n    act. coef.     log act.
-------------------------------------------------------------------------
  NO3-                  0.02613         1617.      0.8505       -1.6531
  Na+                   0.02440         559.7      0.8567       -1.6798
  H+                   0.001051         1.057      0.8813       -3.0332
  Ca++                 0.0003220         12.88      0.5626       -3.7419
  O2(aq)               0.0002506         8.003      1.0069       -3.5980
  SiO2(aq)            6.170e-005         3.699      1.0069       -4.2067
  CaNO3+              3.747e-005         3.817      0.8567       -4.4934
  CO2(aq)             1.116e-005        0.4900      1.0000       -4.9524
   (only species > 1e-8 molal listed)

 Mineral saturation states
                    log Q/K                            log Q/K
-------------------------------------------------------------------
  Quartz            -0.2074        Cristobalite      -0.7579
  Tridymite         -0.3732        Amrph^silica      -1.4931
  Chalcedony        -0.4786
   (only minerals with log Q/K > -3 listed)

 Gases                 fugacity      log fug.
-------------------------------------------------
  O2(g)                   0.2000      -0.699
  Steam                  0.03131      -1.504
  CO2(g)               0.0003162      -3.500
  N2(g)               1.169e-005      -4.932
  H2(g)               6.282e-042     -41.202
  CH4(g)              3.888e-146    -145.410

                                  In fluid              Sorbed             Kd
 Original basis total moles   moles     mg/kg      moles     mg/kg      L/kg
-------------------------------------------------------------------------------
---
  Ca++            0.000360   0.000360      14.4
  H+               0.00106    0.00106      1.07
  H2O                 55.5       55.5 9.98e+005
  HCO3-           1.12e-005  1.12e-005     0.680
  NO3-               0.0262     0.0262 1.62e+003
  Na+                0.0244     0.0244      560.
  O2(aq)           0.000251   0.000251      8.00
  SiO2(aq)        6.17e-005  6.17e-005      3.70
```

15) BASIN 3 CHEMISTRY AFTER ALKALINE DISCHARGE FROM BASIN 2, FLASH MIX RATIO=0.079

```
      Step #    79             Xi = 0.0790
          Temperature =  25.0 C    Pressure =  1.013 bars
```

```
        pH =  3.050              log fO2 =   -0.699
        Eh =   1.0382 volts      pe =  17.5512
        Ionic strength      =    0.026239
        Activity of water   =    1.000000
        Solvent mass        =    1.000000 kg
        Solution mass       =    1.002193 kg
        Solution density    =    1.014    g/cm3
        Chlorinity          =    0.000000 molal
        Dissolved solids    =        2188 mg/kg sol'n
        Elect. conductivity =     2552.55 uS/cm (or umho/cm)
        Hardness            =       36.95 mg/kg sol'n as CaCO3
          carbonate         =        0.00 mg/kg sol'n as CaCO3
          non-carbonate     =       36.95 mg/kg sol'n as CaCO3
        Rock mass           =    0.000000 kg
        Carbonate alkalinity=        0.00 mg/kg sol'n as CaCO3
        Water type          =    Na-NO3
```

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			
Ca++	0.0004476	3.839e-005	0.001539	
H+	0.0005314	4.558e-005	4.594e-005	
H2O	51.12	4.385	79.00	
NO3-	0.02146	0.001841	0.1141	
Na+	0.02008	0.001722	0.03959	
O2(g)	-- fixed fugacity buffer --			
SiO2(aq)	6.558e-005	5.625e-006	0.0003380	

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
NO3-	0.02591	1603.	0.8510	-1.6566
Na+	0.02419	555.0	0.8572	-1.6832
H+	0.001012	1.017	0.8816	-3.0497
Ca++	0.0003316	13.26	0.5636	-3.7284
O2(aq)	0.0002507	8.003	1.0068	-3.5980
SiO2(aq)	6.245e-005	3.744	1.0068	-4.2015
CaNO3+	3.833e-005	3.904	0.8572	-4.4834
CO2(aq)	1.116e-005	0.4900	1.0000	-4.9524

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Quartz	-0.2022	Cristobalite	-0.7527
Tridymite	-0.3680	Amrph^silica	-1.4879
Chalcedony	-0.4734		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.2000	-0.699
Steam	0.03131	-1.504
CO2(g)	0.0003162	-3.500
N2(g)	1.066e-005	-4.972

```
   H2(g)               6.282e-042     -41.202
   CH4(g)              3.888e-146    -145.410

                                    In fluid              Sorbed            Kd
  Original basis total moles   moles     mg/kg      moles     mg/kg      L/kg
 ----------------------------------------------------------------------------
---
   Ca++            0.000370   0.000370      14.8
   H+               0.00102    0.00102      1.03
   H2O                 55.5       55.5 9.98e+005
   HCO3-          1.12e-005  1.12e-005     0.680
   NO3-               0.0259     0.0259 1.61e+003
   Na+                0.0242     0.0242      555.
   O2(aq)           0.000251   0.000251      8.00
   SiO2(aq)        6.25e-005  6.25e-005      3.74
```

16) BASIN 3 CHEMISTRY AFTER ACIDIC DISCHARGE FROM BASIN 2, FLASH MIX RATIO=0.335

```
       Step #   335             Xi = 0.3350
          Temperature =  25.0 C    Pressure =  1.013 bars
          pH =  3.031              log fO2 =   -0.699
          Eh =   1.0394 volts      pe =  17.5699
          Ionic strength      =    0.026361
          Activity of water   =    1.000000
          Solvent mass        =    1.000000 kg
          Solution mass       =    1.002202 kg
          Solution density    =    1.014    g/cm3
          Chlorinity          =    0.000000 molal
          Dissolved solids    =        2198 mg/kg sol'n
          Elect. conductivity =     2571.78 uS/cm (or umho/cm)
          Hardness            =       37.12 mg/kg sol'n as CaCO3
            carbonate         =        0.00 mg/kg sol'n as CaCO3
            non-carbonate     =       37.12 mg/kg sol'n as CaCO3
          Rock mass           =    0.000000 kg
          Carbonate alkalinity=        0.00 mg/kg sol'n as CaCO3
          Water type          =    Na-NO3

                           moles        moles         grams          cm3
  Reactants             remaining     reacted       reacted       reacted
 ----------------------------------------------------------------------------
   CO2(g)              -- fixed fugacity buffer --
   Ca++                 0.0002494     0.0001256      0.005035
   H+                   0.0007647     0.0003853     0.0003883
   H2O                      36.91         18.60         335.0
   NO3-                   0.01749      0.008810        0.5463
   Na+                    0.01623      0.008174        0.1879
   O2(g)               -- fixed fugacity buffer --
   SiO2(aq)            4.103e-005    2.067e-005      0.001242

  No minerals in system.

  Aqueous species       molality    mg/kg sol'n    act. coef.     log act.
 ----------------------------------------------------------------------------
   NO3-                   0.02603         1610.      0.8508       -1.6548
   Na+                    0.02427         556.7      0.8569       -1.6820
   H+                    0.001056         1.062      0.8815       -3.0311
```

```
   Ca++                 0.0003330         13.32      0.5630       -3.7270
   O2(aq)               0.0002506         8.003      1.0068       -3.5980
   SiO2(aq)            6.223e-005         3.731      1.0068       -4.2030
   CaNO3+              3.863e-005         3.935      0.8569       -4.4801
   CO2(aq)             1.116e-005        0.4900      1.0000       -4.9524
    (only species > 1e-8 molal listed)

  Mineral saturation states
                     log Q/K                                log Q/K
 ------------------------------------------------------------------
   Quartz            -0.2037       Cristobalite      -0.7542
   Tridymite         -0.3695       Amrph^silica      -1.4894
   Chalcedony        -0.4749
    (only minerals with log Q/K > -3 listed)

  Gases                fugacity      log fug.
 ------------------------------------------------
   O2(g)                  0.2000      -0.699
   Steam                 0.03131      -1.504
   CO2(g)               0.0003162      -3.500
   N2(g)               1.172e-005      -4.931
   H2(g)               6.282e-042     -41.202
   CH4(g)              3.888e-146    -145.410

                                   In fluid              Sorbed            Kd
  Original basis total moles   moles     mg/kg      moles     mg/kg      L/kg
 ------------------------------------------------------------------------------
---
   Ca++            0.000372   0.000372      14.9
   H+               0.00107    0.00107      1.07
   H2O                 55.5       55.5 9.98e+005
   HCO3-           1.12e-005  1.12e-005     0.680
   NO3-               0.0261     0.0261 1.61e+003
   Na+                0.0243     0.0243      557.
   O2(aq)           0.000251   0.000251      8.00
   SiO2(aq)        6.22e-005  6.22e-005      3.73
```

17) BASIN 3 CHEMISTRY AFTER ALKALINE DISCHARGE FROM BASIN 2, FLASH MIX RATIO=0.079

```
    Step #    79             Xi = 0.0790
          Temperature =  25.0 C    Pressure =  1.013 bars
          pH =  3.046              log fO2 =   -0.699
          Eh =   1.0385 volts      pe =  17.5552
          Ionic strength      =    0.026187
          Activity of water   =    1.000000
          Solvent mass        =    1.000000 kg
          Solution mass       =    1.002188 kg
          Solution density    =    1.014    g/cm3
          Chlorinity          =    0.000000 molal
          Dissolved solids    =        2183 mg/kg sol'n
          Elect. conductivity =     2549.74 uS/cm (or umho/cm)
          Hardness            =       38.05 mg/kg sol'n as CaCO3
            carbonate         =        0.00 mg/kg sol'n as CaCO3
            non-carbonate     =       38.05 mg/kg sol'n as CaCO3
          Rock mass           =    0.000000 kg
          Carbonate alkalinity=        0.00 mg/kg sol'n as CaCO3
```

Water type = Na-NO3

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			
Ca++	0.0004476	3.839e-005	0.001539	
H+	0.0005314	4.558e-005	4.594e-005	
H2O	51.12	4.385	79.00	
NO3-	0.02146	0.001841	0.1141	
Na+	0.02008	0.001722	0.03959	
O2(g)	-- fixed fugacity buffer --			
SiO2(aq)	6.558e-005	5.625e-006	0.0003380	

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
NO3-	0.02585	1599.	0.8511	-1.6576
Na+	0.02410	552.9	0.8573	-1.6848
H+	0.001021	1.027	0.8817	-3.0457
Ca++	0.0003416	13.66	0.5638	-3.7153
O2(aq)	0.0002507	8.003	1.0068	-3.5980
SiO2(aq)	6.291e-005	3.772	1.0068	-4.1983
CaNO3+	3.940e-005	4.014	0.8573	-4.4713
CO2(aq)	1.116e-005	0.4900	1.0000	-4.9524

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Quartz	-0.1990	Cristobalite	-0.7495
Tridymite	-0.3648	Amrph^silica	-1.4847
Chalcedony	-0.4702		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.2000	-0.699
Steam	0.03131	-1.504
CO2(g)	0.0003162	-3.500
N2(g)	1.081e-005	-4.966
H2(g)	6.282e-042	-41.202
CH4(g)	3.888e-146	-145.410

		In fluid		Sorbed		Kd
Original basis	total moles	moles	mg/kg	moles	mg/kg	L/kg
Ca++	0.000381	0.000381	15.2			
H+	0.00103	0.00103	1.04			
H2O	55.5	55.5	9.98e+005			
HCO3-	1.12e-005	1.12e-005	0.680			
NO3-	0.0259	0.0259	1.60e+003			
Na+	0.0241	0.0241	553.			
O2(aq)	0.000251	0.000251	8.00			
SiO2(aq)	6.29e-005	6.29e-005	3.77			

18) BASIN 3 CHEMISTRY AFTER ACIDIC DISCHARGE FROM BASIN 2, FLASH MIX RATIO=0.335

```
          Step #   335             Xi = 0.3350
          Temperature =  25.0 C    Pressure =  1.013 bars
          pH =  3.028              log fO2 =   -0.699
          Eh =   1.0395 volts      pe =  17.5726
          Ionic strength      =    0.026322
          Activity of water   =    1.000000
          Solvent mass        =    1.000000 kg
          Solution mass       =    1.002198 kg
          Solution density    =    1.014    g/cm3
          Chlorinity          =    0.000000 molal
          Dissolved solids    =        2194 mg/kg sol'n
          Elect. conductivity =     2569.66 uS/cm (or umho/cm)
          Hardness            =       37.85 mg/kg sol'n as CaCO3
            carbonate         =        0.00 mg/kg sol'n as CaCO3
            non-carbonate     =       37.85 mg/kg sol'n as CaCO3
          Rock mass           =    0.000000 kg
          Carbonate alkalinity=        0.00 mg/kg sol'n as CaCO3
          Water type          =    Na-NO3
```

Reactants	moles remaining	moles reacted	grams reacted	cm3 reacted
CO2(g)	-- fixed fugacity buffer --			
Ca++	0.0002494	0.0001256	0.005035	
H+	0.0007647	0.0003853	0.0003883	
H2O	36.91	18.60	335.0	
NO3-	0.01749	0.008810	0.5463	
Na+	0.01623	0.008174	0.1879	
O2(g)	-- fixed fugacity buffer --			
SiO2(aq)	4.103e-005	2.067e-005	0.001242	

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
NO3-	0.02598	1607.	0.8508	-1.6555
Na+	0.02420	555.1	0.8570	-1.6832
H+	0.001063	1.069	0.8815	-3.0283
Ca++	0.0003396	13.58	0.5632	-3.7183
O2(aq)	0.0002507	8.003	1.0068	-3.5980
SiO2(aq)	6.250e-005	3.747	1.0068	-4.2012
CaNO3+	3.934e-005	4.007	0.8570	-4.4722
CO2(aq)	1.116e-005	0.4900	1.0000	-4.9524

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Quartz	-0.2019	Cristobalite	-0.7524
Tridymite	-0.3677	Amrph^silica	-1.4876
Chalcedony	-0.4731		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.

```
 ------------------------------------------------
   O2(g)                   0.2000      -0.699
   Steam                  0.03131      -1.504
   CO2(g)               0.0003162      -3.500
   N2(g)                1.183e-005      -4.927
   H2(g)                6.282e-042     -41.202
   CH4(g)               3.888e-146    -145.410

                                  In fluid              Sorbed            Kd
  Original basis total moles   moles     mg/kg      moles     mg/kg      L/kg
 ------------------------------------------------------------------------------
---
   Ca++             0.000379   0.000379      15.2
   H+                0.00107    0.00107      1.08
   H2O                  55.5       55.5 9.98e+005
   HCO3-            1.12e-005  1.12e-005     0.680
   NO3-                0.0260     0.0260 1.61e+003
   Na+                 0.0242     0.0242      555.
   O2(aq)           0.000251   0.000251      8.00
   SiO2(aq)        6.25e-005  6.25e-005      3.75
```

19) BASIN 3 CHEMISTRY AFTER ALKALINE DISCHARGE FROM BASIN 2, FLASH MIX RATIO=0.079

```
  Step #    79             Xi = 0.0790
         Temperature =  25.0 C    Pressure =  1.013 bars
         pH =  3.046              log fO2 =   -0.699
         Eh =   1.0385 volts      pe =  17.5553
         Ionic strength      =    0.026114
         Activity of water   =    1.000000
         Solvent mass        =    1.000000 kg
         Solution mass       =    1.002181 kg
         Solution density    =    1.014    g/cm3
         Chlorinity          =    0.000000 molal
         Dissolved solids    =        2176 mg/kg sol'n
         Elect. conductivity =     2543.50 uS/cm (or umho/cm)
         Hardness            =       38.70 mg/kg sol'n as CaCO3
           carbonate         =        0.00 mg/kg sol'n as CaCO3
           non-carbonate     =       38.70 mg/kg sol'n as CaCO3
         Rock mass           =    0.000000 kg
         Carbonate alkalinity=        0.00 mg/kg sol'n as CaCO3
         Water type          =    Na-NO3

                          moles        moles         grams          cm3
  Reactants             remaining     reacted       reacted       reacted
 ------------------------------------------------------------------------------
   CO2(g)              -- fixed fugacity buffer --
   Ca++                 0.0004476    3.839e-005      0.001539
   H+                   0.0005314    4.558e-005    4.594e-005
   H2O                      51.12         4.385         79.00
   NO3-                   0.02146      0.001841        0.1141
   Na+                    0.02008      0.001722       0.03959
   O2(g)               -- fixed fugacity buffer --
   SiO2(aq)            6.558e-005    5.625e-006     0.0003380

  No minerals in system.
```

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
NO3-	0.02577	1594.	0.8513	-1.6589
Na+	0.02401	550.8	0.8574	-1.6864
H+	0.001021	1.027	0.8818	-3.0457
Ca++	0.0003475	13.90	0.5642	-3.7077
O2(aq)	0.0002507	8.004	1.0068	-3.5980
SiO2(aq)	6.319e-005	3.788	1.0068	-4.1964
CaNO3+	3.998e-005	4.073	0.8574	-4.4649
CO2(aq)	1.116e-005	0.4900	1.0000	-4.9524

(only species > 1e-8 molal listed)

Mineral saturation states

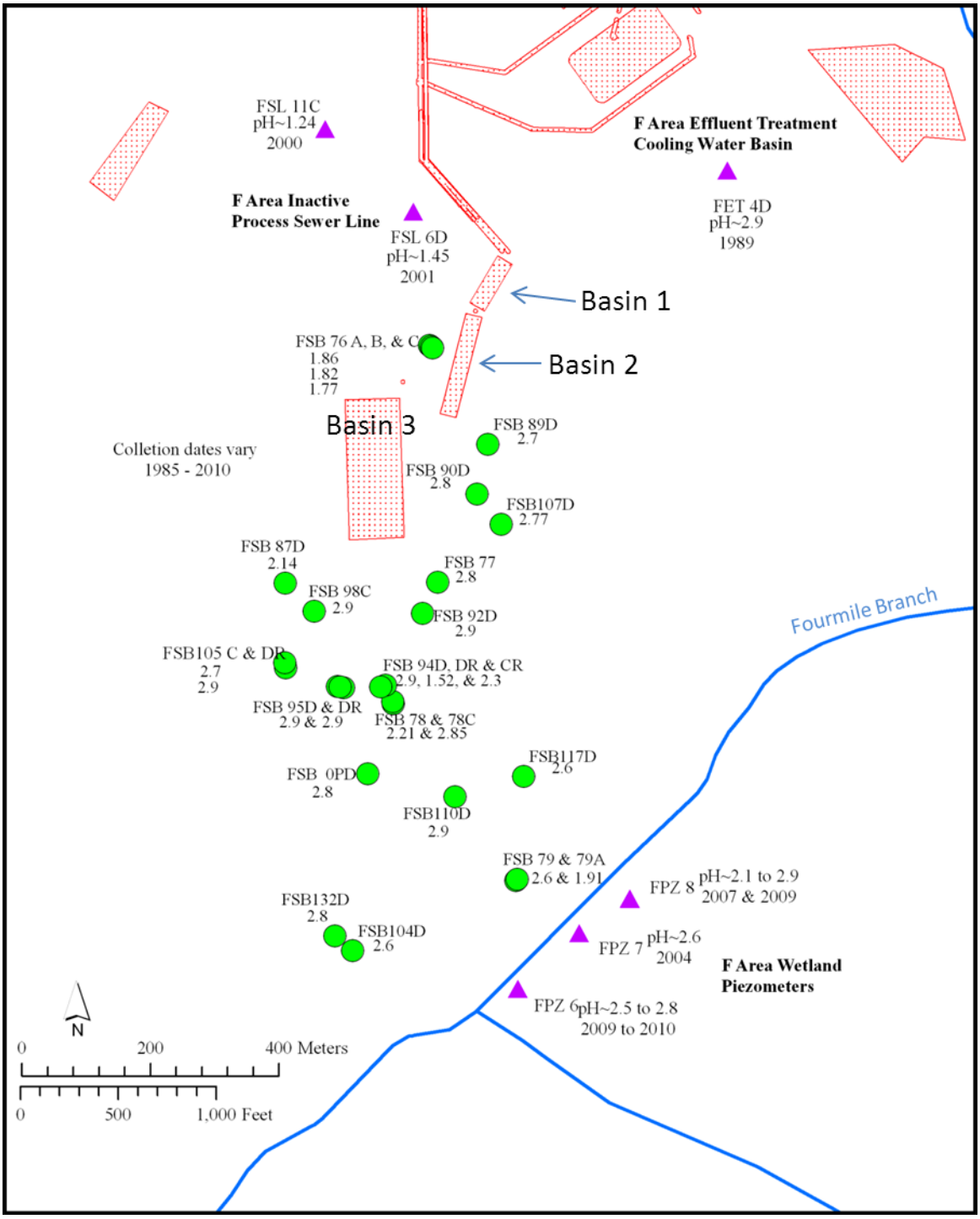
	log Q/K		log Q/K
Quartz	-0.1971	Cristobalite	-0.7476
Tridymite	-0.3629	Amrph^silica	-1.4828
Chalcedony	-0.4683		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.2000	-0.699
Steam	0.03131	-1.504
CO2(g)	0.0003162	-3.500
N2(g)	1.075e-005	-4.969
H2(g)	6.282e-042	-41.202
CH4(g)	3.888e-146	-145.410

		In fluid		Sorbed		Kd
Original basis	total moles	moles	mg/kg	moles	mg/kg	L/kg
Ca++	0.000387	0.000387	15.5			
H+	0.00103	0.00103	1.04			
H2O	55.5	55.5	9.98e+005			
HCO3-	1.12e-005	1.12e-005	0.680			
NO3-	0.0258	0.0258	1.60e+003			
Na+	0.0240	0.0240	551.			
O2(aq)	0.000251	0.000251	8.00			
SiO2(aq)	6.32e-005	6.32e-005	3.79			

APPENDIX D: GROUNDWATER PH



Data from the ERDMS database. Green circles represent groundwater pH data collected from 1985 through 2010. Purple triangles show pH and collected date. Only pH measurements <3.0 are shown on the map.

pH Data for FSB78

Date	pH	Source
10/1/1981	well installed	Killian et al. 1985
3/1/1982	2.7	Killian et al. 1985
5/20/1982	3.1	Killian et al. 1985
7/21/1982	2.9	Killian et al. 1985
10/6/1982	2.8	Killian et al. 1985
1/5/1983	2.7	Killian et al. 1985
4/7/1983	2.4	Killian et al. 1985
9/28/1983	2.3	Killian et al. 1985
12/15/1983	3.2	Killian et al. 1985
2/13/1984	4.2	Killian et al. 1985
4/19/1984	4.1	Killian et al. 1985
7/3/1984 9:15	2.9	ERDMS database
10/1/1984 11:18	3.3	ERDMS database
2/19/1985 10:03	3.2	ERDMS database
2/21/1985 11:47	3.2	ERDMS database
4/1/1985 10:12	3.3	ERDMS database
4/9/1985 10:15	3.4	ERDMS database
7/1/1985 12:29	2.7	ERDMS database
9/25/1985 8:56	3	ERDMS database
1/20/1986 11:11	2.8	ERDMS database
4/21/1986 10:39	3.1	ERDMS database
7/27/1986 12:00	3	ERDMS database
7/29/1986 13:00	3.6	ERDMS database
10/18/1986 11:45	2.9	ERDMS database
1/6/1987 15:40	3	ERDMS database
4/2/1987 10:50	3	ERDMS database
7/28/1987 12:30	3.5	ERDMS database
1/23/1988 11:35	3	ERDMS database
4/5/1988 9:55	3.3	ERDMS database
4/23/1988 14:15	3	ERDMS database
7/9/1988 7:35	2.9	ERDMS database
10/8/1988 16:55	2.9	ERDMS database
2/25/1989 13:35	3.1	ERDMS database
5/22/1989 15:55	3.1	ERDMS database
7/1/1989 11:45	2.9	ERDMS database
10/10/1989 14:20	2.9	ERDMS database
1/6/1990 10:50	2.7	ERDMS database
4/24/1990 18:05	2.9	ERDMS database
6/13/1990 13:30	3	ERDMS database
7/12/1990 13:50	3	ERDMS database
9/26/1990 14:45	3.1	ERDMS database
10/1/1990 13:30	3.2	ERDMS database

*Note: Table only includes data through 1990; seepage basins were capped ~1990

APPENDIX E: BASIN 3 CHEMISTRY AT PH 2.7, 2.9, 3.0, 3.2, AND 3.4

BASIN 3 CHEMISTRY AT pH 2.7

```
        Temperature =  25.0 C    Pressure =  1.013 bars
        pH =  2.700              log fO2 =   -0.699
        Eh =   1.0589 volts      pe =  17.9010
        Ionic strength      =    0.032615
        Solution density    =    1.014    g/cm3
        Dissolved solids    =        2675 mg/kg sol'n
        Elect. conductivity =     3286.72 uS/cm (or umho/cm)

 No minerals in system.
```

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
NO3-	0.03157	1952.	0.8380	-1.5775
Na+	0.02916	668.7	0.8453	-1.6081
H+	0.002284	2.296	0.8737	-2.6999
O2(aq)	0.0002502	7.986	1.0085	-3.5980
SO4--	0.0001958	18.75	0.5058	-4.0043
Ca++	0.0001255	5.015	0.5371	-4.1715
Cl-	5.044e-005	1.783	0.8380	-4.3740
SiO2(aq)	4.444e-005	2.663	1.0085	-4.3485
FeOH++	4.256e-005	3.092	0.5219	-4.6534
Al+++	4.226e-005	1.137	0.2895	-4.9124
Fe+++	2.368e-005	1.319	0.2895	-5.1640
HSO4-	2.300e-005	2.227	0.8453	-4.7112
CaNO3+	1.681e-005	1.712	0.8453	-4.8474
NaSO4-	1.427e-005	1.694	0.8453	-4.9186
K+	1.412e-005	0.5506	0.8380	-4.9269
CO2(aq)	1.116e-005	0.4898	1.0000	-4.9524
FeSO4+	1.038e-005	1.572	0.8453	-5.0569
Fe(OH)2+	4.365e-006	0.3912	0.8453	-5.4330
UO2++	3.855e-006	1.038	0.5219	-5.6964
FeNO3++	3.473e-006	0.4082	0.5219	-5.7417
AlSO4+	1.465e-006	0.1798	0.8453	-5.9071
CaSO4	1.394e-006	0.1892	1.0000	-5.8558
AlOH++	1.366e-007	0.005992	0.5219	-7.1470
UO2SO4	1.115e-007	0.04072	1.0000	-6.9526
Fe2(OH)2++++	1.027e-007	0.01493	0.1291	-7.8775
FeH3SiO4++	7.646e-008	0.01151	0.5219	-7.3990
N2(aq)	5.020e-008	0.001403	1.0000	-7.2993
NaCl	2.621e-008	0.001528	1.0000	-7.5815
Fe(SO4)2-	1.931e-008	0.004775	0.8453	-7.7873
CaCl+	1.689e-008	0.001272	0.8453	-7.8454
FeCl++	1.676e-008	0.001526	0.5219	-8.0580
FeHSO4++	1.310e-008	0.001998	0.5219	-8.1652
Al(SO4)2-	1.135e-008	0.002480	0.8453	-8.0180
KSO4-	9.870e-009	0.001330	0.8453	-8.0787
UO2OH+	9.667e-009	0.002767	0.8453	-8.0877
HCO3-	2.837e-009	0.0001726	0.8487	-8.6185
UO2(NO3)2	1.150e-009	0.0004518	1.0000	-8.9394
Fe(OH)3	8.277e-010	8.822e-005	1.0000	-9.0821
UO2(SO4)2--	6.933e-010	0.0003195	0.5058	-9.4551

Al(OH)2+	2.864e-010	1.742e-005	0.8453	-9.6160
Fe3(OH)4(5+)	2.505e-010	5.884e-005	0.0407	-10.9914
UO2SiO(OH)3+	2.173e-010	7.913e-005	0.8453	-9.7360
UO2Cl+	1.727e-010	5.261e-005	0.8453	-9.8357
Fe++	1.651e-010	9.194e-006	0.5371	-10.0523
NaHCO3	7.987e-011	6.692e-006	1.0000	-10.0976
H2SO4	3.834e-011	3.750e-006	1.0000	-10.4163
KCl	1.293e-011	9.612e-007	1.0000	-10.8885
Al2(OH)2++++	6.166e-012	5.410e-007	0.1291	-12.0992
OH-	6.137e-012	1.041e-007	0.8417	-11.2869
H3SiO4-	4.127e-012	3.914e-007	0.8453	-11.4574
(UO2)2(OH)2++	4.071e-012	2.331e-006	0.5219	-11.6727
CaHCO3+	3.170e-012	3.196e-007	0.8532	-11.5679
FeCO3+	2.319e-012	2.680e-007	0.8453	-11.7077
FeCl2+	1.955e-012	2.472e-007	0.8453	-11.7818
FeSO4	1.390e-012	2.106e-007	1.0000	-11.8569
NaH3SiO4	1.213e-012	1.428e-007	1.0000	-11.9162
UO2CO3	4.909e-013	1.616e-007	1.0000	-12.3090
Al(OH)3	1.049e-013	8.159e-009	1.0000	-12.9793
NaOH	7.993e-014	3.188e-009	1.0000	-13.0973
HCl	6.700e-014	2.436e-009	1.0000	-13.1739
FeCl+	1.063e-014	9.677e-010	0.8453	-14.0466
CaOH+	8.181e-015	4.658e-010	0.8453	-14.1602
CaH3SiO4+	5.198e-015	7.008e-010	0.8453	-14.3572
HNO2	2.686e-015	1.259e-010	1.0000	-14.5710
NO2-	9.661e-016	4.433e-011	0.8380	-15.0917
Fe(OH)4-	1.156e-016	1.428e-011	0.8453	-16.0100
CO3--	1.063e-016	6.363e-012	0.5140	-16.2624
Al(OH)4-	6.363e-017	6.029e-012	0.8453	-16.2693
Al3(OH)4(5+)	3.902e-017	5.797e-012	0.0407	-17.7989
KOH	1.940e-017	1.086e-012	1.0000	-16.7122
FeNO2++	1.508e-017	1.532e-012	0.5219	-17.1039
FeCl3	6.977e-018	1.129e-012	1.0000	-17.1563
CaCO3	6.054e-018	6.043e-013	1.0000	-17.2180
NaCO3-	5.090e-018	4.214e-013	0.8453	-17.3663
FeHCO3+	5.033e-018	5.866e-013	0.8453	-17.3712
FeOH+	3.480e-018	2.529e-013	0.8453	-17.5314
(UO2)3(OH)4++	1.299e-018	1.138e-012	0.5219	-18.1687
FeCl2	1.993e-019	2.519e-014	1.0000	-18.7005
(UO2)3(OH)5+	4.618e-020	4.122e-014	0.8453	-19.4086
(UO2)2(CO3)(OH)3	2.176e-021	1.413e-015	0.8453	-20.7354
UO2+	1.827e-021	4.919e-016	0.8453	-20.8113
UO2(CO3)2--	1.426e-021	5.547e-016	0.5058	-21.1419
CaH2SiO4	6.740e-022	9.020e-017	1.0000	-21.1713
H2SiO4--	2.755e-022	2.586e-017	0.5058	-21.8559
FeCO3	2.320e-023	2.681e-018	1.0000	-22.6344
Ca(H3SiO4)2	1.165e-023	2.675e-018	1.0000	-22.9339
FeCl4-	4.198e-024	8.275e-019	0.8453	-23.4500
H6(H2SiO4)4--	7.372e-026	2.812e-020	0.5058	-25.4284
(UO2)4(OH)7+	1.943e-026	2.324e-020	0.8453	-25.7845
Fe(OH)2	8.421e-027	7.547e-022	1.0000	-26.0746
(UO2)3(OH)7-	3.512e-027	3.255e-021	0.8453	-26.5274
ClO4-	6.226e-028	6.175e-023	0.8417	-27.2806
UO2(CO3)3----	2.529e-032	1.135e-026	0.0649	-32.7850
Fe(OH)3-	7.870e-037	8.388e-032	0.8453	-36.1770
U(OH)2++	2.233e-040	6.059e-035	0.5219	-39.9335
U(OH)3+	1.625e-040	4.686e-035	0.8453	-39.8620

UOH+++	3.380e-041	8.597e-036	0.2754	-41.0311
U(OH)4	1.525e-041	4.654e-036	1.0000	-40.8168
H4(H2SiO4)4----	7.279e-042	2.762e-036	0.0649	-42.3259
U(SO4)2	4.540e-042	1.948e-036	1.0000	-41.3430
USO4++	4.534e-042	1.511e-036	0.5219	-41.6259
U++++	6.420e-043	1.524e-037	0.1291	-43.0816
H2(aq)	4.813e-045	9.676e-042	1.0085	-44.3139
UCl+++	2.744e-046	7.485e-041	0.2754	-46.1216
U(OH)5-	9.825e-047	3.166e-041	0.8453	-46.0807
NH4+	2.316e-053	4.166e-049	0.8342	-52.7141
NH4SO4-	1.970e-056	2.241e-051	0.8453	-55.7786
NH3	5.111e-060	8.681e-056	1.0000	-59.2915
UCl4	2.557e-061	9.688e-056	1.0000	-60.5922
U+++	5.257e-070	1.248e-064	0.2754	-69.8393

Mineral saturation states

	log Q/K		log Q/K
Uranophane	25.3014s/sat	Tridymite	-0.5150
Hematite	5.8284s/sat	Chalcedony	-0.6204
Nontronit-Na	2.8075s/sat	Cristobalite	-0.8997
Nontronit-Ca	2.7090s/sat	Amrph^silica	-1.6349
Goethite	2.4360s/sat	Fe(OH)3(ppd)	-1.9531
Nontronit-K	2.0423s/sat	UO2SO4^3H2O	-2.1741
Quartz	-0.3492		

(only minerals with log Q/K > -3 listed)

BASIN 3 CHEMISTRY AT pH 2.9

Temperature = 25.0 C Pressure = 1.013 bars
pH = 2.900 log fO2 = -0.699
Eh = 1.0471 volts pe = 17.7012
Ionic strength = 0.028807
Solution density = 1.014 g/cm3
Dissolved solids = 2370 mg/kg sol'n
Elect. conductivity = 2815.74 uS/cm (or umho/cm)

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
NO3-	0.02779	1719.	0.8455	-1.6290
Na+	0.02601	596.6	0.8521	-1.6543
H+	0.001434	1.442	0.8783	-2.8997
Ca++	0.0002516	10.06	0.5522	-3.8572
O2(aq)	0.0002505	7.996	1.0075	-3.5980
SO4--	0.0001549	14.84	0.5230	-4.0915
Cl-	9.986e-005	3.532	0.8455	-4.0735
SiO2(aq)	5.582e-005	3.346	1.0075	-4.2500
FeOH++	3.766e-005	2.737	0.5380	-4.6933
Al+++	3.187e-005	0.8579	0.3042	-5.0134
CaNO3+	3.054e-005	3.110	0.8521	-4.5846
Fe+++	1.298e-005	0.7231	0.3042	-5.4036
HSO4-	1.178e-005	1.141	0.8521	-4.9983

CO2(aq)	1.116e-005	0.4899	1.0000	-4.9524
K+	1.062e-005	0.4141	0.8455	-5.0469
NaSO4-	1.041e-005	1.236	0.8521	-5.0521
Fe(OH)2+	6.258e-006	0.5610	0.8521	-5.2730
FeSO4+	4.849e-006	0.7348	0.8521	-5.3838
UO2++	2.907e-006	0.7831	0.5380	-5.8057
CaSO4	2.350e-006	0.3192	1.0000	-5.6289
FeNO3++	1.723e-006	0.2026	0.5380	-6.0328
AlSO4+	9.422e-007	0.1156	0.8521	-6.0954
AlOH++	1.663e-007	0.007300	0.5380	-7.0482
FeH3SiO4++	8.491e-008	0.01279	0.5380	-7.3402
Fe2(OH)2++++	7.923e-008	0.01152	0.1393	-7.9572
UO2SO4	7.091e-008	0.02590	1.0000	-7.1493
CaCl+	6.899e-008	0.005199	0.8521	-7.2307
NaCl	4.708e-008	0.002745	1.0000	-7.3272
FeCl++	1.871e-008	0.001704	0.5380	-7.9972
N2(aq)	1.578e-008	0.0004411	1.0000	-7.8018
UO2OH+	1.181e-008	0.003381	0.8521	-7.9973
Fe(SO4)2-	7.379e-009	0.001825	0.8521	-8.2015
KSO4-	6.076e-009	0.0008192	0.8521	-8.2859
Al(SO4)2-	5.969e-009	0.001305	0.8521	-8.2936
HCO3-	4.459e-009	0.0002714	0.8552	-8.4187
FeHSO4++	3.778e-009	0.0005764	0.5380	-8.6919
Fe(OH)3	1.895e-009	0.0002020	1.0000	-8.7224
UO2(NO3)2	7.052e-010	0.0002772	1.0000	-9.1517
Al(OH)2+	5.650e-010	3.438e-005	0.8521	-9.3175
UO2(SO4)2--	3.487e-010	0.0001608	0.5230	-9.7390
UO2SiO(OH)3+	3.331e-010	0.0001213	0.8521	-9.5470
Fe3(OH)4(5+)	2.674e-010	6.285e-005	0.0459	-10.9112
UO2Cl+	2.660e-010	8.107e-005	0.8521	-9.6446
Fe++	1.465e-010	8.160e-006	0.5522	-10.0922
NaHCO3	1.138e-010	9.535e-006	1.0000	-9.9440
KCl	1.959e-011	1.457e-006	1.0000	-10.7079
H2SO4	1.250e-011	1.223e-006	1.0000	-10.9032
CaHCO3+	1.028e-011	1.037e-006	0.8594	-11.0539
OH-	9.640e-012	1.636e-007	0.8489	-11.0871
Al2(OH)2++++	9.004e-012	7.903e-007	0.1393	-11.9017
H3SiO4-	8.137e-012	7.721e-007	0.8521	-11.1590
(UO2)2(OH)2++	5.988e-012	3.429e-006	0.5380	-11.4919
FeCl2+	4.457e-012	5.636e-007	0.8521	-11.4204
FeCO3+	3.325e-012	3.843e-007	0.8521	-11.5477
NaH3SiO4	2.168e-012	2.554e-007	1.0000	-11.6640
FeSO4	1.038e-012	1.572e-007	1.0000	-11.9840
UO2CO3	9.577e-013	3.153e-007	1.0000	-12.0188
Al(OH)3	3.304e-013	2.571e-008	1.0000	-12.4809
NaOH	1.138e-013	4.543e-009	1.0000	-12.9437
HCl	8.449e-014	3.073e-009	1.0000	-13.0732
CaOH+	2.650e-014	1.509e-009	0.8521	-13.6462
CaH3SiO4+	2.113e-014	2.850e-009	0.8521	-13.7446
FeCl+	1.921e-014	1.750e-009	0.8521	-13.7859
HNO2	1.506e-015	7.063e-011	1.0000	-14.8222
NO2-	8.505e-016	3.904e-011	0.8455	-15.1432
Fe(OH)4-	4.159e-016	5.140e-011	0.8521	-15.4505
Al(OH)4-	3.150e-016	2.986e-011	0.8521	-15.5712
CO3--	2.585e-016	1.547e-011	0.5306	-15.8628
Al3(OH)4(5+)	1.085e-016	1.613e-011	0.0459	-17.3028
FeCl3	3.203e-017	5.183e-012	1.0000	-16.4945

CaCO3	3.132e-017	3.128e-012	1.0000	-16.5042
KOH	2.332e-017	1.305e-012	1.0000	-16.6323
NaCO3-	1.139e-017	9.434e-013	0.8521	-17.0128
FeNO2++	7.485e-018	7.606e-013	0.5380	-17.3950
FeHCO3+	7.215e-018	8.412e-013	0.8521	-17.2112
FeOH+	4.989e-018	3.626e-013	0.8521	-17.3714
(UO2)3(OH)4++	3.728e-018	3.266e-012	0.5380	-17.6977
FeCl2	7.255e-019	9.174e-014	1.0000	-18.1394
(UO2)3(OH)5+	2.147e-019	1.917e-013	0.8521	-18.7377
(UO2)2(CO3)(OH)3	1.301e-020	8.451e-015	0.8521	-19.9552
UO2(CO3)2--	6.752e-021	2.627e-015	0.5230	-20.4521
CaH2SiO4	4.376e-021	5.858e-016	1.0000	-20.3589
UO2+	2.231e-021	6.011e-016	0.8521	-20.7209
H2SiO4--	8.391e-022	7.877e-017	0.5230	-21.3577
Ca(H3SiO4)2	9.487e-023	2.180e-017	1.0000	-22.0229
FeCO3	5.313e-023	6.140e-018	1.0000	-22.2747
FeCl4-	3.818e-023	7.529e-018	0.8521	-22.4876
H6(H2SiO4)4--	4.437e-025	1.693e-019	0.5230	-24.6345
(UO2)4(OH)7+	1.762e-025	2.108e-019	0.8521	-24.8235
(UO2)3(OH)7-	4.098e-026	3.798e-020	0.8521	-25.4570
Fe(OH)2	1.928e-026	1.728e-021	1.0000	-25.7149
ClO4-	1.233e-027	1.224e-022	0.8489	-26.9801
UO2(CO3)3----	2.716e-031	1.220e-025	0.0742	-31.6956
Fe(OH)3-	2.832e-036	3.019e-031	0.8521	-35.6175
U(OH)3+	1.986e-040	5.726e-035	0.8521	-39.7716
U(OH)2++	1.684e-040	4.570e-035	0.5380	-40.0429
H4(H2SiO4)4----	9.936e-041	3.771e-035	0.0742	-41.1324
U(OH)4	2.975e-041	9.082e-036	1.0000	-40.5266
UOH+++	1.572e-041	4.000e-036	0.2905	-41.3403
USO4++	1.114e-042	3.714e-037	0.5380	-42.2222
U(SO4)2	9.408e-043	4.037e-037	1.0000	-42.0265
U++++	1.843e-043	4.376e-038	0.1393	-43.5906
H2(aq)	4.818e-045	9.689e-042	1.0075	-44.3139
U(OH)5-	3.012e-046	9.708e-041	0.8521	-45.5906
UCl+++	1.610e-046	4.392e-041	0.2905	-46.3301
NH4+	8.120e-054	1.461e-049	0.8420	-53.1651
NH4SO4-	5.657e-057	6.439e-052	0.8521	-56.3169
NH3	2.866e-060	4.869e-056	1.0000	-59.5428
UCl4	1.261e-060	4.780e-055	1.0000	-59.8992
Al13O4(OH)24(7+)	3.421e-069	2.808e-063	0.0024	-71.0902
U+++	2.445e-070	5.806e-065	0.2905	-70.1485

Mineral saturation states

	log Q/K		log Q/K
Uranophane	26.7928s/sat	Tridymite	-0.4165
Hematite	6.5479s/sat	Chalcedony	-0.5219
Nontronit-Na	4.1040s/sat	Cristobalite	-0.8012
Nontronit-Ca	4.0726s/sat	Amrph^silica	-1.5364
Nontronit-K	3.3144s/sat	Fe(OH)3(ppd)	-1.5934
Goethite	2.7957s/sat	UO2SO4^3H2O	-2.3708
Quartz	-0.2507		

(only minerals with log Q/K > -3 listed)

BASIN 3 CHEMISTRY AT pH 3.0

```
          Temperature =  25.0 C    Pressure =  1.013 bars
          pH =  3.000              log fO2 =   -0.699
          Eh =   1.0412 volts      pe =  17.6013
          Ionic strength      =    0.027478
          Solution density    =    1.014    g/cm3
          Dissolved solids    =        2264 mg/kg sol'n
          Elect. conductivity =     2648.76 uS/cm (or umho/cm)
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
NO3-	0.02648	1638.	0.8483	-1.6486
Na+	0.02491	571.4	0.8547	-1.6718
H+	0.001137	1.144	0.8800	-2.9997
Ca++	0.0002963	11.85	0.5580	-3.7816
O2(aq)	0.0002506	8.000	1.0071	-3.5980
SO4--	0.0001397	13.39	0.5295	-4.1310
Cl-	0.0001171	4.142	0.8483	-4.0029
SiO2(aq)	5.979e-005	3.584	1.0071	-4.2203
FeOH++	3.485e-005	2.534	0.5441	-4.7220
CaNO3+	3.464e-005	3.528	0.8547	-4.5286
Al+++	2.823e-005	0.7599	0.3099	-5.0581
CO2(aq)	1.116e-005	0.4900	1.0000	-4.9524
Fe+++	9.474e-006	0.5279	0.3099	-5.5323
K+	9.397e-006	0.3666	0.8483	-5.0985
NaSO4-	9.104e-006	1.081	0.8547	-5.1090
HSO4-	8.522e-006	0.8253	0.8547	-5.1377
Fe(OH)2+	7.351e-006	0.6590	0.8547	-5.2019
FeSO4+	3.283e-006	0.4975	0.8547	-5.5520
UO2++	2.575e-006	0.6936	0.5441	-5.8536
CaSO4	2.554e-006	0.3470	1.0000	-5.5927
FeNO3++	1.211e-006	0.1424	0.5441	-6.1811
AlSO4+	7.739e-007	0.09500	0.8547	-6.1795
AlOH++	1.868e-007	0.008197	0.5441	-6.9930
CaCl+	9.630e-008	0.007257	0.8547	-7.0846
FeH3SiO4++	8.414e-008	0.01267	0.5441	-7.3393
Fe2(OH)2++++	6.744e-008	0.009804	0.1433	-8.0148
UO2SO4	5.800e-008	0.02118	1.0000	-7.2366
NaCl	5.320e-008	0.003102	1.0000	-7.2741
FeCl++	1.618e-008	0.001474	0.5441	-8.0553
UO2OH+	1.327e-008	0.003801	0.8547	-7.9452
N2(aq)	9.102e-009	0.0002544	1.0000	-8.0409
HCO3-	5.597e-009	0.0003407	0.8577	-8.3187
KSO4-	4.912e-009	0.0006623	0.8547	-8.3770
Fe(SO4)2-	4.562e-009	0.001129	0.8547	-8.4091
Al(SO4)2-	4.477e-009	0.0009786	0.8547	-8.4172
Fe(OH)3	2.810e-009	0.0002996	1.0000	-8.5513
FeHSO4++	2.015e-009	0.0003075	0.5441	-8.9599
Al(OH)2+	8.052e-010	4.900e-005	0.8547	-9.1623
UO2(NO3)2	5.771e-010	0.0002269	1.0000	-9.2388
UO2SiO(OH)3+	4.009e-010	0.0001460	0.8547	-9.4652
UO2Cl+	2.794e-010	8.517e-005	0.8547	-9.6219
Fe3(OH)4(5+)	2.638e-010	6.201e-005	0.0480	-10.8975

UO2(SO4)2--	2.573e-010	0.0001186	0.5295	-9.8658
NaHCO3	1.376e-010	1.153e-005	1.0000	-9.8615
Fe++	1.357e-010	7.559e-006	0.5580	-10.1209
KCl	2.046e-011	1.522e-006	1.0000	-10.6890
CaHCO3+	1.536e-011	1.549e-006	0.8617	-10.8784
OH-	1.210e-011	2.052e-007	0.8516	-10.9871
Al2(OH)2++++	1.128e-011	9.905e-007	0.1433	-11.7912
H3SiO4-	1.093e-011	1.038e-006	0.8547	-11.0294
(UO2)2(OH)2++	7.525e-012	4.310e-006	0.5441	-11.3878
H2SO4	7.203e-012	7.048e-007	1.0000	-11.1425
FeCl2+	4.572e-012	5.782e-007	0.8547	-11.4081
FeCO3+	3.905e-012	4.514e-007	0.8547	-11.4766
NaH3SiO4	2.806e-012	3.306e-007	1.0000	-11.5519
UO2CO3	1.359e-012	4.475e-007	1.0000	-11.8668
FeSO4	8.867e-013	1.344e-007	1.0000	-12.0522
Al(OH)3	5.945e-013	4.627e-008	1.0000	-12.2259
NaOH	1.377e-013	5.493e-009	1.0000	-12.8612
HCl	7.896e-014	2.872e-009	1.0000	-13.1026
CaOH+	3.958e-014	2.255e-009	0.8547	-13.4707
CaH3SiO4+	3.379e-014	4.558e-009	0.8547	-13.5393
FeCl+	2.109e-014	1.921e-009	0.8547	-13.7442
HNO2	1.144e-015	5.364e-011	1.0000	-14.9418
NO2-	8.103e-016	3.719e-011	0.8483	-15.1628
Fe(OH)4-	7.740e-016	9.566e-011	0.8547	-15.1795
Al(OH)4-	7.112e-016	6.742e-011	0.8547	-15.2162
CO3--	4.047e-016	2.423e-011	0.5369	-15.6630
Al3(OH)4(5+)	1.913e-016	2.844e-011	0.0480	-17.0371
CaCO3	5.906e-017	5.898e-012	1.0000	-16.2287
FeCl3	3.876e-017	6.273e-012	1.0000	-16.4116
KOH	2.606e-017	1.459e-012	1.0000	-16.5840
NaCO3-	1.729e-017	1.432e-012	0.8547	-16.8305
FeHCO3+	8.474e-018	9.881e-013	0.8547	-17.1401
(UO2)3(OH)4++	6.649e-018	5.825e-012	0.5441	-17.4415
FeOH+	5.860e-018	4.260e-013	0.8547	-17.3003
FeNO2++	5.260e-018	5.345e-013	0.5441	-17.5433
FeCl2	9.395e-019	1.188e-013	1.0000	-18.0271
(UO2)3(OH)5+	4.859e-019	4.339e-013	0.8547	-18.3817
(UO2)2(CO3)(OH)3	3.288e-020	2.136e-014	0.8547	-19.5513
UO2(CO3)2--	1.499e-020	5.835e-015	0.5295	-20.1003
CaH2SiO4	8.835e-021	1.183e-015	1.0000	-20.0538
UO2+	2.508e-021	6.757e-016	0.8547	-20.6688
H2SiO4--	1.406e-021	1.320e-016	0.5295	-21.1282
Ca(H3SiO4)2	2.051e-022	4.712e-017	1.0000	-21.6881
FeCO3	7.877e-023	9.106e-018	1.0000	-22.1036
FeCl4-	5.419e-023	1.069e-017	0.8547	-22.3342
H6(H2SiO4)4--	9.125e-025	3.482e-019	0.5295	-24.3159
(UO2)4(OH)7+	5.659e-025	6.771e-019	0.8547	-24.3154
(UO2)3(OH)7-	1.469e-025	1.362e-019	0.8547	-24.9011
Fe(OH)2	2.859e-026	2.563e-021	1.0000	-25.5438
ClO4-	1.446e-027	1.435e-022	0.8516	-26.9096
UO2(CO3)3----	9.205e-031	4.133e-025	0.0780	-31.1440
Fe(OH)3-	5.269e-036	5.618e-031	0.8547	-35.3465
H4(H2SiO4)4----	3.119e-040	1.184e-034	0.0780	-40.6140
U(OH)3+	2.232e-040	6.436e-035	0.8547	-39.7195
U(OH)2++	1.491e-040	4.048e-035	0.5441	-40.0907
U(OH)4	4.221e-041	1.289e-035	1.0000	-40.3746
UOH+++	1.097e-041	2.791e-036	0.2964	-41.4881

USO4++	5.688e-043	1.896e-037	0.5441	-42.5093
U(SO4)2	4.435e-043	1.903e-037	1.0000	-42.3531
U++++	1.012e-043	2.404e-038	0.1433	-43.8383
H2(aq)	4.819e-045	9.693e-042	1.0071	-44.3139
U(OH)5-	5.364e-046	1.729e-040	0.8547	-45.3387
UCl+++	1.049e-046	2.863e-041	0.2964	-46.5072
NH4+	4.882e-054	8.787e-050	0.8449	-53.3846
NH4SO4-	3.107e-057	3.537e-052	0.8547	-56.5759
NH3	2.176e-060	3.698e-056	1.0000	-59.6623
UCl4	1.365e-060	5.174e-055	1.0000	-59.8648
Al13O4(OH)24(7+)	1.295e-066	1.063e-060	0.0026	-68.4738
U+++	1.706e-070	4.051e-065	0.2964	-70.2963

Mineral saturation states

	log Q/K		log Q/K
Uranophane	27.4316s/sat	Tridymite	-0.3868
Hematite	6.8901s/sat	Chalcedony	-0.4922
Nontronit-Na	4.6665s/sat	Cristobalite	-0.7715
Nontronit-Ca	4.6533s/sat	Fe(OH)3(ppd)	-1.4223
Nontronit-K	3.8656s/sat	Amrph^silica	-1.5067
Goethite	2.9668s/sat	UO2SO4^3H2O	-2.4581
Quartz	-0.2210		

(only minerals with log Q/K > -3 listed)

BASIN 3 CHEMISTRY AT pH 3.2

Temperature = 25.0 C Pressure = 1.013 bars
pH = 3.200 log fO2 = -0.699
Eh = 1.0294 volts pe = 17.4009
Ionic strength = 0.025590
Solution density = 1.014 g/cm3
Dissolved solids = 2113 mg/kg sol'n
Elect. conductivity = 2408.86 uS/cm (or umho/cm)

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
NO3-	0.02461	1523.	0.8525	-1.6782
Na+	0.02335	535.7	0.8585	-1.6979
H+	0.0007148	0.7189	0.8825	-3.2001
Ca++	0.0003607	14.43	0.5666	-3.6896
O2(aq)	0.0002507	8.005	1.0066	-3.5980
Cl-	0.0001415	5.007	0.8525	-3.9185
SO4--	0.0001171	11.22	0.5392	-4.1997
SiO2(aq)	6.544e-005	3.923	1.0066	-4.1813
CaNO3+	3.981e-005	4.056	0.8585	-4.4662
FeOH++	2.900e-005	2.108	0.5533	-4.7946
Al+++	2.301e-005	0.6194	0.3186	-5.1349
CO2(aq)	1.116e-005	0.4900	1.0000	-4.9524
Fe(OH)2+	9.822e-006	0.8808	0.8585	-5.0741
K+	7.663e-006	0.2990	0.8525	-5.1849
NaSO4-	7.285e-006	0.8655	0.8585	-5.2038
Fe+++	4.914e-006	0.2739	0.3186	-5.8053
HSO4-	4.566e-006	0.4422	0.8585	-5.4067

CaSO4	2.695e-006	0.3662	1.0000	-5.5694
UO2++	2.099e-006	0.5656	0.5533	-5.9350
FeSO4+	1.488e-006	0.2256	0.8585	-5.8937
FeNO3++	5.933e-007	0.06977	0.5533	-6.4837
AlSO4+	5.512e-007	0.06767	0.8585	-6.3250
AlOH++	2.442e-007	0.01072	0.5533	-6.8693
CaCl+	1.440e-007	0.01085	0.8585	-6.9080
FeH3SiO4++	7.657e-008	0.01153	0.5533	-7.3729
NaCl	6.084e-008	0.003548	1.0000	-7.2158
Fe2(OH)2++++	4.625e-008	0.006724	0.1496	-8.1600
UO2SO4	4.105e-008	0.01500	1.0000	-7.3867
UO2OH+	1.738e-008	0.004978	0.8585	-7.8262
FeCl++	1.031e-008	0.0009391	0.5533	-8.2439
HCO3-	8.841e-009	0.0005383	0.8613	-8.1183
Fe(OH)3	5.983e-009	0.0006380	1.0000	-8.2231
KSO4-	3.421e-009	0.0004614	0.8585	-8.5321
N2(aq)	3.155e-009	8.820e-005	1.0000	-8.5010
Al(SO4)2-	2.722e-009	0.0005951	0.8585	-8.6314
Fe(SO4)2-	1.765e-009	0.0004368	0.8585	-8.8194
Al(OH)2+	1.690e-009	0.0001029	0.8585	-8.8383
UO2SiO(OH)3+	5.741e-010	0.0002092	0.8585	-9.3073
FeHSO4++	5.688e-010	8.679e-005	0.5533	-9.5020
UO2(NO3)2	4.174e-010	0.0001641	1.0000	-9.3795
UO2Cl+	2.801e-010	8.540e-005	0.8585	-9.6189
Fe3(OH)4(5+)	2.370e-010	5.572e-005	0.0513	-10.9149
NaHCO3	2.055e-010	1.722e-005	1.0000	-9.6873
UO2(SO4)2--	1.526e-010	7.039e-005	0.5392	-10.0846
Fe++	1.130e-010	6.299e-006	0.5666	-10.1935
CaHCO3+	2.999e-011	3.026e-006	0.8651	-10.5859
KCl	2.037e-011	1.516e-006	1.0000	-10.6910
Al2(OH)2++++	1.910e-011	1.677e-006	0.1496	-11.5440
OH-	1.910e-011	3.242e-007	0.8555	-10.7867
H3SiO4-	1.889e-011	1.793e-006	0.8585	-10.7900
(UO2)2(OH)2++	1.280e-011	7.333e-006	0.5533	-11.1498
FeCO3+	5.218e-012	6.033e-007	0.8585	-11.3488
NaH3SiO4	4.585e-012	5.403e-007	1.0000	-11.3387
FeCl2+	3.582e-012	4.531e-007	0.8585	-11.5121
UO2CO3	2.835e-012	9.338e-007	1.0000	-11.5474
H2SO4	2.443e-012	2.391e-007	1.0000	-11.6120
Al(OH)3	1.989e-012	1.548e-007	1.0000	-11.7014
FeSO4	6.405e-013	9.708e-008	1.0000	-12.1935
NaOH	2.056e-013	8.206e-009	1.0000	-12.6870
CaOH+	7.728e-014	4.402e-009	0.8585	-13.1782
CaH3SiO4+	7.217e-014	9.735e-009	0.8585	-13.2079
HCl	6.046e-014	2.200e-009	1.0000	-13.2185
FeCl+	2.158e-014	1.966e-009	0.8585	-13.7323
Al(OH)4-	3.758e-015	3.563e-010	0.8585	-14.4913
Fe(OH)4-	2.603e-015	3.218e-010	0.8585	-14.6508
CO3--	1.001e-015	5.993e-011	0.5464	-15.2622
NO2-	7.531e-016	3.457e-011	0.8525	-15.1925
HNO2	6.732e-016	3.158e-011	1.0000	-15.1718
Al3(OH)4(5+)	6.665e-016	9.909e-011	0.0513	-16.4659
CaCO3	1.837e-016	1.835e-011	1.0000	-15.7358
NaCO3-	4.078e-017	3.378e-012	0.8585	-16.4558
FeCl3	3.705e-017	5.997e-012	1.0000	-16.4312
KOH	3.388e-017	1.897e-012	1.0000	-16.4700
(UO2)3(OH)4++	2.360e-017	2.068e-011	0.5533	-16.8842

FeHCO3+	1.132e-017	1.321e-012	0.8585	-17.0123
FeOH+	7.831e-018	5.693e-013	0.8585	-17.1725
(UO2)3(OH)5+	2.769e-018	2.474e-012	0.8585	-17.6239
FeNO2++	2.577e-018	2.619e-013	0.5533	-17.8460
FeCl2	1.173e-018	1.483e-013	1.0000	-17.9308
(UO2)2(CO3)(OH)3	2.260e-019	1.469e-013	0.8585	-18.7121
UO2(CO3)2--	7.730e-020	3.009e-014	0.5392	-19.3800
CaH2SiO4	3.006e-020	4.025e-015	1.0000	-19.5220
H2SiO4--	3.801e-021	3.569e-016	0.5392	-20.6884
UO2+	3.284e-021	8.849e-016	0.8585	-20.5499
Ca(H3SiO4)2	7.634e-022	1.754e-016	1.0000	-21.1173
FeCO3	1.677e-022	1.939e-017	1.0000	-21.7754
FeCl4-	6.265e-023	1.236e-017	0.8585	-22.2693
(UO2)4(OH)7+	6.730e-024	8.053e-018	0.8585	-23.2383
H6(H2SiO4)4--	3.229e-024	1.232e-018	0.5392	-23.7592
(UO2)3(OH)7-	2.108e-024	1.954e-018	0.8585	-23.7424
Fe(OH)2	6.087e-026	5.458e-021	1.0000	-25.2156
ClO4-	1.748e-027	1.735e-022	0.8555	-26.8251
UO2(CO3)3----	1.130e-029	5.075e-024	0.0839	-30.0229
Fe(OH)3-	1.772e-035	1.890e-030	0.8585	-34.8178
H4(H2SiO4)4----	2.627e-039	9.974e-034	0.0839	-39.6565
U(OH)3+	2.922e-040	8.429e-035	0.8585	-39.6006
U(OH)2++	1.216e-040	3.301e-035	0.5533	-40.1721
U(OH)4	8.807e-041	2.690e-035	1.0000	-40.0552
UOH+++	5.562e-042	1.416e-036	0.3054	-41.7699
USO4++	1.573e-043	5.244e-038	0.5533	-43.0603
U(SO4)2	1.065e-043	4.571e-038	1.0000	-42.9727
U++++	3.195e-044	7.588e-039	0.1496	-44.3206
H2(aq)	4.822e-045	9.699e-042	1.0066	-44.3139
U(OH)5-	1.767e-045	5.698e-040	0.8585	-44.8189
UCl+++	4.075e-047	1.112e-041	0.3054	-46.9050
NH4+	1.803e-054	3.245e-050	0.8493	-53.8151
NH4SO4-	9.800e-058	1.116e-052	0.8585	-57.0750
NH3	1.281e-060	2.177e-056	1.0000	-59.8924
UCl4	9.792e-061	3.712e-055	1.0000	-60.0091
Al13O4(OH)24(7+)	2.951e-061	2.424e-055	0.0030	-63.0588
U+++	8.651e-071	2.055e-065	0.3054	-70.5781

Mineral saturation states

	log Q/K		log Q/K
Uranophane	28.6412s/sat	Tridymite	-0.3478
Hematite	7.5465s/sat	Chalcedony	-0.4532
Nontronit-Ca	5.7071s/sat	Cristobalite	-0.7325
Nontronit-Na	5.6965s/sat	Fe(OH)3(ppd)	-1.0941
Nontronit-K	4.8758s/sat	Amrph^silica	-1.4677
Goethite	3.2950s/sat	UO2SO4^3H2O	-2.6082
Quartz	-0.1820	Jarosite-K	-2.9108

(only minerals with log Q/K > -3 listed)

BASIN 3 CHEMISTRY AT pH 3.2

```
          Temperature =  25.0 C    Pressure =  1.013 bars
          pH =  3.403              log fO2 =   -0.699
          Eh =   1.0174 volts      pe =  17.1984
          Ionic strength      =    0.024393
          Solution density    =    1.014    g/cm3
          Dissolved solids    =        2017 mg/kg sol'n
          Elect. conductivity =     2255.49 uS/cm (or umho/cm)
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
NO3-	0.02343	1450.	0.8552	-1.6982
Na+	0.02236	513.1	0.8610	-1.7154
H+	0.0004476	0.4502	0.8843	-3.4026
Ca++	0.0004019	16.08	0.5724	-3.6382
O2(aq)	0.0002508	8.008	1.0063	-3.5980
Cl-	0.0001570	5.555	0.8552	-3.8720
SO4--	0.0001021	9.788	0.5458	-4.2539
SiO2(aq)	6.901e-005	4.138	1.0063	-4.1583
CaNO3+	4.268e-005	4.348	0.8610	-4.4348
FeOH++	2.323e-005	1.689	0.5595	-4.8862
Al+++	1.964e-005	0.5287	0.3245	-5.1957
Fe(OH)2+	1.264e-005	1.134	0.8610	-4.9631
CO2(aq)	1.116e-005	0.4901	1.0000	-4.9524
K+	6.566e-006	0.2562	0.8552	-5.2506
NaSO4-	6.158e-006	0.7316	0.8610	-5.2756
CaSO4	2.678e-006	0.3638	1.0000	-5.5722
HSO4-	2.521e-006	0.2442	0.8610	-5.6635
Fe+++	2.451e-006	0.1366	0.3245	-6.0993
UO2++	1.793e-006	0.4832	0.5595	-5.9986
FeSO4+	6.653e-007	0.1009	0.8610	-6.2420
AlSO4+	4.216e-007	0.05177	0.8610	-6.4400
AlOH++	3.346e-007	0.01469	0.5595	-6.7277
FeNO3++	2.848e-007	0.03349	0.5595	-6.7977
CaCl+	1.798e-007	0.01355	0.8610	-6.8102
NaCl	6.503e-008	0.003793	1.0000	-7.1869
FeH3SiO4++	6.467e-008	0.009743	0.5595	-7.4415
UO2SO4	3.129e-008	0.01143	1.0000	-7.5046
Fe2(OH)2++++	2.948e-008	0.004287	0.1540	-8.3430
UO2OH+	2.386e-008	0.006834	0.8610	-7.6874
HCO3-	1.405e-008	0.0008558	0.8637	-7.9158
Fe(OH)3	1.231e-008	0.001313	1.0000	-7.9097
FeCl++	5.764e-009	0.0005252	0.5595	-8.4915
Al(OH)2+	3.723e-009	0.0002266	0.8610	-8.4941
KSO4-	2.588e-009	0.0003491	0.8610	-8.6520
Al(SO4)2-	1.838e-009	0.0004019	0.8610	-8.8007
N2(aq)	1.133e-009	3.167e-005	1.0000	-8.9459
UO2SiO(OH)3+	8.310e-010	0.0003028	0.8610	-9.1454
Fe(SO4)2-	6.966e-010	0.0001724	0.8610	-9.2220
UO2(NO3)2	3.288e-010	0.0001293	1.0000	-9.4830
NaHCO3	3.146e-010	2.637e-005	1.0000	-9.5023
UO2Cl+	2.685e-010	8.185e-005	0.8610	-9.6361
Fe3(OH)4(5+)	1.919e-010	4.513e-005	0.0537	-10.9870

FeHSO4++	1.583e-010	2.415e-005	0.5595	-10.0528
UO2(SO4)2--	1.015e-010	4.679e-005	0.5458	-10.2567
Fe++	9.061e-011	5.050e-006	0.5724	-10.2851
CaHCO3+	5.368e-011	5.416e-006	0.8674	-10.3320
Al2(OH)2++++	3.564e-011	3.129e-006	0.1540	-11.2606
H3SiO4-	3.165e-011	3.004e-006	0.8610	-10.5646
OH-	3.035e-011	5.152e-007	0.8582	-10.5842
(UO2)2(OH)2++	2.400e-011	1.375e-005	0.5595	-10.8721
KCl	1.949e-011	1.450e-006	1.0000	-10.7102
NaH3SiO4	7.401e-012	8.723e-007	1.0000	-11.1307
Al(OH)3	7.003e-012	5.451e-007	1.0000	-11.1547
FeCO3+	6.717e-012	7.767e-007	0.8610	-11.2378
UO2CO3	6.223e-012	2.050e-006	1.0000	-11.2060
FeCl2+	2.248e-012	2.843e-007	0.8610	-11.7133
H2SO4	8.487e-013	8.307e-008	1.0000	-12.0713
FeSO4	4.578e-013	6.940e-008	1.0000	-12.3393
NaOH	3.148e-013	1.257e-008	1.0000	-12.5020
CaOH+	1.383e-013	7.877e-009	0.8610	-12.9243
CaH3SiO4+	1.361e-013	1.837e-008	0.8610	-12.9310
HCl	4.221e-014	1.536e-009	1.0000	-13.3746
Al(OH)4-	2.103e-014	1.994e-009	0.8610	-13.7422
FeCl+	1.939e-014	1.767e-009	0.8610	-13.7774
Fe(OH)4-	8.513e-015	1.052e-009	0.8610	-14.1349
Al3(OH)4(5+)	2.703e-015	4.019e-010	0.0537	-15.8383
CO3--	2.514e-015	1.505e-010	0.5527	-14.8572
NO2-	7.170e-016	3.292e-011	0.8552	-15.2124
CaCO3	5.255e-016	5.249e-011	1.0000	-15.2794
HNO2	4.034e-016	1.893e-011	1.0000	-15.3943
NaCO3-	9.924e-017	8.220e-012	0.8610	-16.0683
(UO2)3(OH)4++	9.708e-017	8.507e-011	0.5595	-16.2651
KOH	4.642e-017	2.599e-012	1.0000	-16.3333
FeCl3	2.595e-017	4.200e-012	1.0000	-16.5859
(UO2)3(OH)5+	1.831e-017	1.636e-011	0.8610	-16.8023
FeHCO3+	1.458e-017	1.700e-012	0.8610	-16.9013
FeOH+	1.008e-017	7.329e-013	0.8610	-17.0615
(UO2)2(CO3)(OH)3	1.730e-018	1.124e-012	0.8610	-17.8269
FeNO2++	1.237e-018	1.257e-013	0.5595	-18.1599
FeCl2	1.176e-018	1.488e-013	1.0000	-17.9294
UO2(CO3)2--	4.259e-019	1.658e-013	0.5458	-18.6337
CaH2SiO4	9.066e-020	1.214e-014	1.0000	-19.0426
H2SiO4--	1.006e-020	9.447e-016	0.5458	-20.2604
UO2+	4.508e-021	1.215e-015	0.8610	-20.4110
Ca(H3SiO4)2	2.427e-021	5.578e-016	1.0000	-20.6149
FeCO3	3.452e-022	3.991e-017	1.0000	-21.4620
(UO2)4(OH)7+	9.765e-023	1.169e-016	0.8610	-22.0753
FeCl4-	4.868e-023	9.602e-018	0.8610	-22.3777
(UO2)3(OH)7-	3.541e-023	3.283e-017	0.8610	-22.5159
H6(H2SiO4)4--	1.002e-023	3.823e-018	0.5458	-23.2623
Fe(OH)2	1.253e-025	1.123e-020	1.0000	-24.9022
ClO4-	1.940e-027	1.925e-022	0.8582	-26.7787
UO2(CO3)3----	1.525e-028	6.850e-023	0.0881	-28.8716
Fe(OH)3-	5.796e-035	6.181e-030	0.8610	-34.3019
H4(H2SiO4)4----	1.997e-038	7.581e-033	0.0881	-38.7546
U(OH)3+	4.011e-040	1.157e-034	0.8610	-39.4617
U(OH)4	1.933e-040	5.903e-035	1.0000	-39.7138
U(OH)2++	1.039e-040	2.820e-035	0.5595	-40.2358
UOH+++	2.955e-042	7.521e-037	0.3115	-42.0360

USO4++	4.668e-044	1.556e-038	0.5595	-43.5831
U(SO4)2	2.819e-044	1.210e-038	1.0000	-43.5498
U++++	1.055e-044	2.507e-039	0.1540	-44.7892
U(OH)5-	6.165e-045	1.988e-039	0.8610	-44.2751
H2(aq)	4.823e-045	9.703e-042	1.0063	-44.3139
UCl+++	1.511e-047	4.125e-042	0.3115	-47.3272
NH4+	6.753e-055	1.216e-050	0.8521	-54.2400
Al13O4(OH)24(7+)	1.321e-055	1.085e-049	0.0032	-57.3696
NH4SO4-	3.242e-058	3.691e-053	0.8610	-57.5542
NH3	7.677e-061	1.305e-056	1.0000	-60.1148
UCl4	5.105e-061	1.935e-055	1.0000	-60.2920
U+++	4.596e-071	1.092e-065	0.3115	-70.8442

Mineral saturation states

	log Q/K		log Q/K
Uranophane	29.8263s/sat	Chalcedony	-0.4302
Hematite	8.1734s/sat	Cristobalite	-0.7095
Nontronit-Ca	6.6741s/sat	Fe(OH)3(ppd)	-0.7807
Nontronit-Na	6.6492s/sat	Amrph^silica	-1.4447
Nontronit-K	5.8125s/sat	UO2SO4^3H2O	-2.7261
Goethite	3.6085s/sat	Jarosite-K	-2.7522
Quartz	-0.1590	Gibbsite	-2.9483
Tridymite	-0.3248	Soddyite	-2.9808

(only minerals with log Q/K > -3 listed)