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Geochemical analysis and modeling for an artificial aquifer recharge study in the shallow zone squifer near Pojoaque, New Mexico.

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Geochemical Analysis and Modeling for an Artificial Aquifer Recharge Study in the Shallow Zone Aquifer near Pojoaque, New Mexico

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1.0 Abstract

An artificial aquifer recharge project is currently being evaluated as a component of the Pojoaque Basin Regional Water System as part of the Aamodt Litigation Settlement Act. The purpose of the project is for aquifer storage, with later retrieval as drinking water. The total diversion of San Juan Chama Project Water (SJCPW) for this project is approximately 4,000 acre-feet per year. It should be noted that some of the SJCPW would be treated and put directly into the drinking water system. The goal of this project is to extract the SJCPW from the Rio Grande and pump it into two arroyos, the Arroyo Jocona and an unnamed arroyo. The hope is that the water will reach the shallow aquifer via infiltration. The United States Geological Survey (USGS) performed a geophysical study of the two above-mentioned arroyos near Pojoaque, New Mexico to determine the lithology if SJCPW will infiltrate through the vadose zone and into the shallow aquifer system. The USGS also drilled four borings and completed monitoring wells in two of the borings. The wells were used to collect water levels and water quality samples.

After performing analysis of the groundwater, using both an inductively couple plasma (ICP) and ion chromatography (IC) instruments, and analysis of the sediments using acid digestion and a batch extraction, it was determined that several analytes exceed the United States Environmental Protection Agency Drinking Water Standards. These analytes include aluminum, beryllium, fluoride, iron, and arsenic. All of these analytes are found at concentrations would most likely be able to be treated using standard modern water treatment techniques.

2.0 Introduction

The Pojoaque Pueblo (Pojoaque) has been allotted 4,000 acre feet per year of San Juan Chama Project Water (SJCPW), which they have decided to put to the beneficial use of aquifer storage, for later retrieval as drinking water by the regional water authority. In order to do this Pojoaque would like to extract their water from the Rio Grande River and pump it into two arroyos the Arroyo Jocona (the eastern most arroyo) and an unnamed arroyo (the western most arroyo) (USGS Espanola, 2002). They will then let the water infiltrate through the vadose zone into the aquifer.

The United States Geological Survey (USGS) has performed a geophysical survey, soil borings, infiltration tests, and monitoring well installation to determine lithology and how it may impact the project. The geophysical tests that have been performed include a resistivity test, to determine the depth of the groundwater prior to drilling: along with an infiltration test to determine whether or not the water will infiltrate to the aquifer, borehole analysis from the drill cuttings, and age dating of the groundwater. For this project, as well as the USGS' project, the primary focus will be on the eastern most Arroyo Jocona (study site).

This project has been modeled after several artificial recharge projects that have been performed throughout the United States, and world. Examples of these projects include a couple of projects performed in Kansas (Tappa et al, 2015) and California (Stamos et al, 2013) by the USGS, and a couple of projects performed here in New Mexico by Daniel B. Stephens and Associates which include the Bear Canyon Aquifer Recharge Project (Moore et al, 2009) and the Mariposa Water Reclamation Facility. The above studies all had their own set of issues to overcome. The most common set of issues that these projects had to overcome included water issues and infiltration issues. Water quality issues commonly included high levels of arsenic and other metals that would dissolve at the artificially recharged waters would pass through the vadose zone. This was an issue with both the projects in Kansas (Tappa et al, 2015) and California (Stamos et al, 2013). The project that was performed in California had infiltration issues associated with their project. The issue that this project faced specifically was clogging,

which is when fine-grained materials 'clog' the coarse grained materials of an infiltration gallery. This in turn prevents water from infiltrating down through the vadose zone and into the aquifer. The California project overcame this issue by removing the infiltration gallery and installing injection wells to inject the directly to the aquifer (Stamos et al 2013).

The objective of this project is to model the water quality of the SJCPW as it infiltrates through the vadose zone of the Tesuque Formation into the aquifer, with the final intention of this project being to determine whether or not the mixture of the SJCPW and aquifer water will be suitable for human consumption.

3.0 Statement of Problem

With the intended use of this water being drinking water, determining the future quality of the shallow aquifer water is important. Located directly east of the subject site are two uranium-mining districts. In July 1954 uranium-containing minerals were discovered in the Santa Fe Group southeast of Espanola, NM (Chenoweth, 1979). As a result of this discovery the area east of Pojoaque, NM was heavily prospected, and hundreds of claims were established (Chenoweth, 1979). These discoveries lead to the creation of two mining districts in the area: the San Jose and Nambe Mining Districts. The San Jose Mining District is located directly east of US Highway 285, approximately 0.5 miles east of the study site, in Pojoaque, NM. The Nambe Mining District is located approximately 10 miles east of the study area. There are 31 mines registered with the New Mexico Bureau of Geology and Mineral Resources (NMBGMR) in the San Juan Mining District; and there are 10 mines registered in the Nambe Mining District (McLemore et al, 2011). However, there are hundreds of prospects between the two mining districts (Chenoweth, 1979). The nearest registered mine to the study site is the Anomaly #9 Mine, located two miles to the east. There are currently no active mines in the project area, and there are no known economically viable ore deposits in either the San Jose or Nambe mining districts (McLemore et al, 2011). It is estimated that 8,754 metric tons of low-grade uranium ore were mined from both the San Jose and Nambe Mining Districts (Chenoweth, 1979).

The sandstone uranium occurrences in the Tesuque Formation likely represent natural precipitation and concentration from uraniferous groundwaters. It is hypothesized that these groundwaters are derived from one or more of three sources: 1) volcanic ash beds found interbedded within the Tesuque Formation, 2) the alteration of granitic and volcanic detritus within the sedimentary host rocks and, 3) veins, replacements, and pegmatites found in the Proterozoic rocks in the Sangre de Cristo Mountains to the east (McLemore et al, 2011). It is further hypothesized that the uranium in modern groundwater is derived from the same sources, as well as the oxidization and leaching of older uranium occurrences in the Tesuque Formation (McLemore et al, 2011). Green clays, granites, and volcanic ash beds have all been shown to contain uranium at detectable levels within the Tesuque Formation (McLemore et al, 2011).

While the study area is located near two mining districts, the water quality from the shallow zone aquifer is relatively unknown for this area. However, there are known issues in the deep zone aquifer include uranium, arsenic, and fluoride (Wolf, 2014). The United States Environmental Protection Agency (USEPA) Safe Drinking Water Program regulates these compounds at 0.03 milligrams per liter (mg/L), 0.01 mg/L, and 4 mg/L respectively. The analytical data for the groundwater in the deep showed these compounds exceeding the USEPA Drinking Water Standards (Wolf, 2014). Nearby domestic production wells, within 1 mile of the study site, have shown detections of uranium ranging from 3.59 mg/L to 5.67 mg/L (McLemore et al, 2011), which exceed the USEPA drinking water standard for uranium.

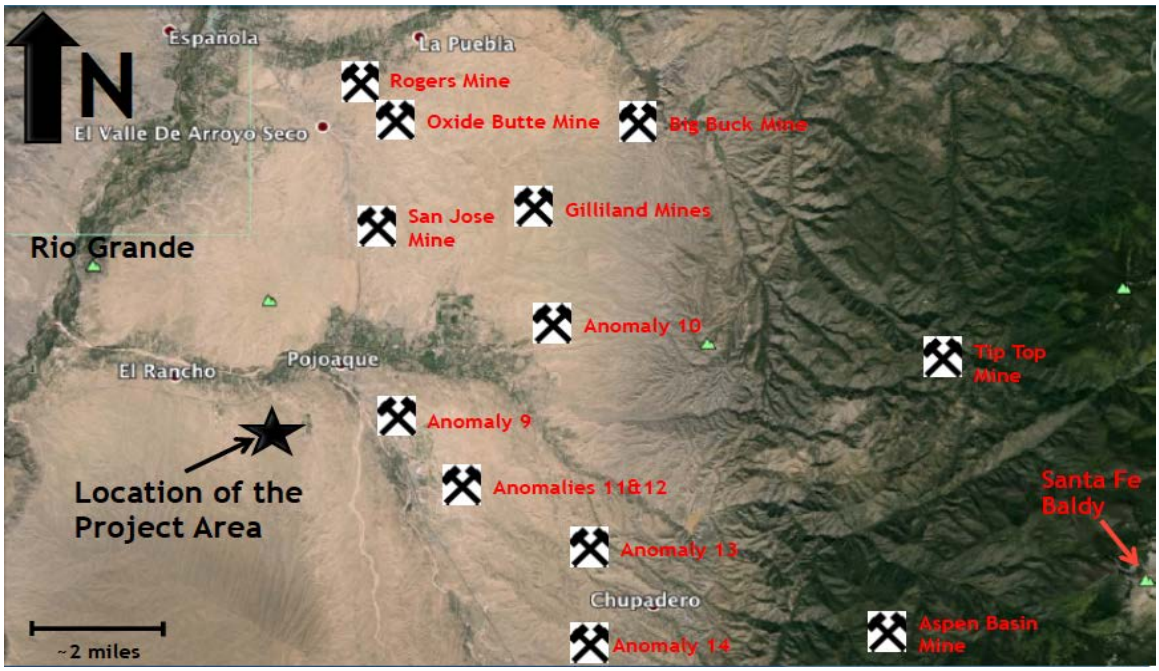


Figure 1: Location of Uranium Mines near the Project Area (Google Earth, modified)

If any of the above-mentioned compounds were to exceed the USEPA Drinking Water Standards, then adverse health effects could be experienced within the exposed population. Health effects from arsenic include skin problems, circulatory system problems, and an increased cancer risk. Health effects from uranium include an increased cancer risk and potential kidney damage. While health effects from fluoride include bone disease, and the potential of children getting mottled teeth. See the Discussion Section for a more detailed description of potential health effects, and ways of removing the contaminants of concern from the drinking water supply.

4.0 Study Area

The study area for this project is located in two arroyos west of U.S. Highway 285-84 and south of NM Highway 502. The area primarily consists of high desert terrain, with vegetation consisting of a piñon-juniper mix. The altitude of the study area ranges from approximately 5,900 feet to approximately 6,050 feet above mean sea level (amsl). The climate of the region is fairly dry and mild. The mean temperature is 51.6°F

(10.8°C), with the average annual precipitation being 9.88 inches (WRCC, 2014). See Figure 3 for a Site Location Map.

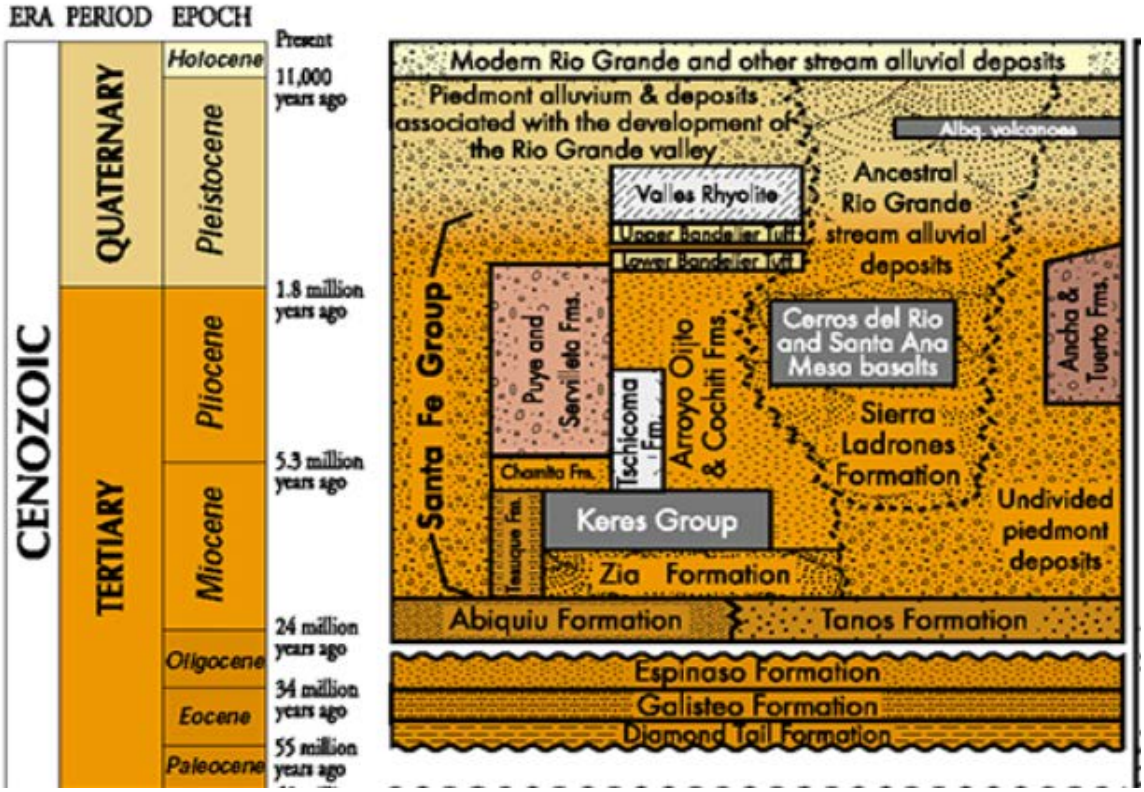


Figure 2: Stratigraphy of the Project Area

The study area is located in the southern part of the Espanola Basin, which is located in northern New Mexico, and is 45 kilometers (28 miles) long and 60 kilometers (37 miles) wide. The sediments within the Espanola Basin consist primarily of the Santa Fe Group. The Santa Fe Group consists of approximately 1,000 meters to 5,000 meters of interbedded sand, silt, clay, and gravel layers (Koning et al, 2005). The portion of the Santa Fe Group that underlies the study site is the Tesuque Formation. The Tesuque Formation is a Miocene aged formation that consists of the Pojoaque, Skull Ridge, and Nambe members. The ages of these members range from 8 million to 20 million years old (Manley, 1978).

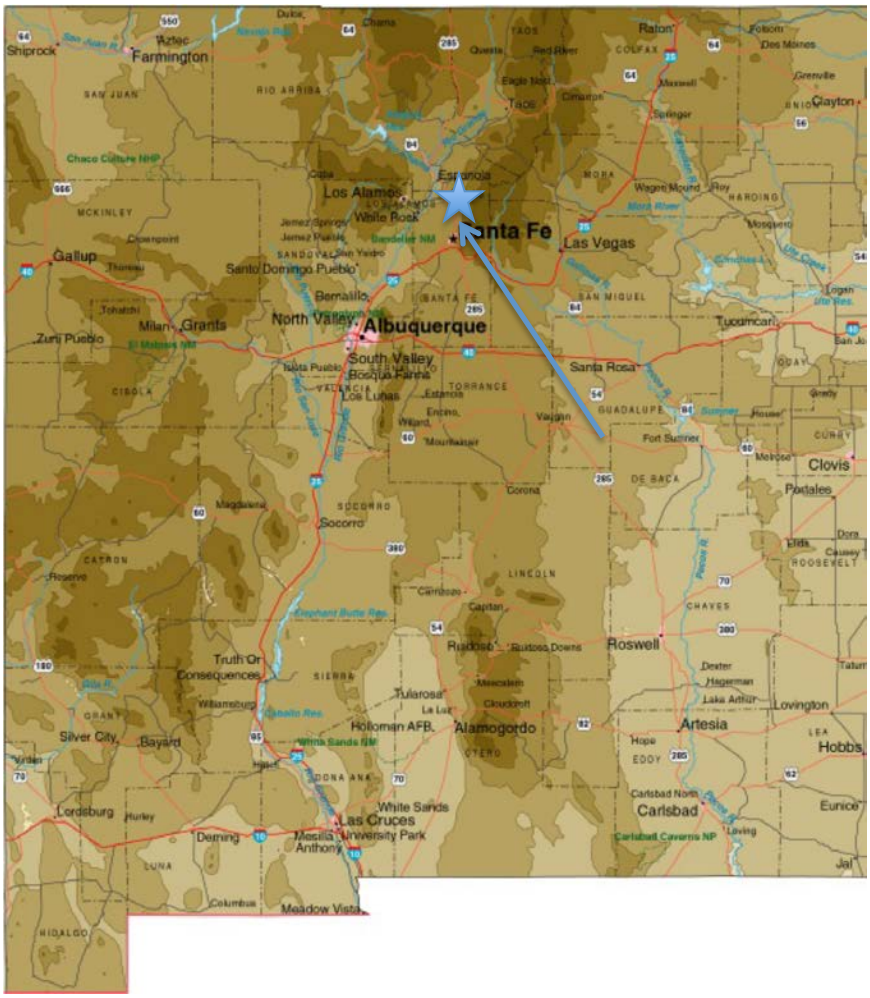


Figure 3: Location of the Project Area. Arrow is pointed towards to the Project Area.

The groundwater depth ranges from 40 feet below ground surface (bgs) to 109 feet bgs (USGS, 2014) for the shallow aquifer, which is the aquifer concerned with in this study. Studies have shown that the Tesuque formation's saturated zone ranges from 100 feet to over 250 feet thick (Wilson et al, 1974).

The Rio Tesuque, Rio Nambe, and the Rio Pojoaque are the primary recharge sources of the deep groundwater beneath the study site. Both the Rio Nambe and the Rio Tesuque are tributaries of the Rio Pojoaque. The headwaters for these three rivers are located in the Santa Fe Mountains (Southern Sangre de Cristo Range), which are located 15 to 20 miles to the east-southeast of the study site. The calculated recharge from the above mentioned rivers into the Tesuque Formations saturated zone is approximately

14,700 acre feet per year, or about 13% of the annual precipitation, which falls in the nearby Santa Fe Mountains (Wasiolek, 1995). There is the possibility of the Rio Pojoaque and the shallow zone aquifer having connectivity. With the increase in aquifer volume "upstream" of the Rio Nambe, the possibility exists of creating an inflow to the river from the aquifer. However, this isn't likely to occur since this stretch of the Pojoaque River is considered to be a losing stream (Rieland et al, 1974).

The Rio Grande, the source of the SJCPW for this project, is located approximately 5 miles to the west of the study site. The headwaters of the Rio Grande River are located in the San Juan Mountains (Southwest Colorado), approximately 150 miles to the northwest of the study area. The Rio Grande flows 220 miles to the confluence with the Rio Chama. The SJCPW originates south of Pagosa Springs, Colorado approximately 100 miles northwest of the study area. A series of diversions are located on each the Rio Blanco, Navajo, and the Little Navajo Rivers before being transferred into the Azotea Tunnel for transportation under the Continental Divide into the Rio Chama. Once in the Rio Chama the water flows for approximately 100 miles to the confluence with the Rio Grande, before flowing another 13 miles to the anticipated extraction point for this project. Once the water is collected from the Rio Grande it will be transported approximately 5 miles east into the arroyos located within the study area.

5.0 Work Plan

The work plan for this project involved several different objectives. The first task was data collection, which involved performing a literature review. This involved the collection of data about the study site and/or information about similar studies from previously performed studies. This involved searching through various academic libraries including the USGS, the NMGS, and/or Google Scholar.

The next facet of this project was the collection of environmental, water and soil, samples from the aquifer and the vadose zone above the aquifer. Water samples were collected using USGS protocols (USGS, variously dated) in order to ensure sample integrity. Monitoring wells were sampled by purging three casing volumes using a

Grundfos Rediflo submersible pump with dedicated polyethylene tubing. Samples were placed into new polyethylene sample bottles and preserved using trace metal grade nitric acid. Samples collected for metals and cations were filtered using a 0.45μm filter. After collection the samples were chilled until it was time for analysis. Soil samples were collected directly from the split spoon augers, at which time the samples were placed into appropriate sample containers. As with the water samples the soil samples were collected using USGS protocols (USGS, variously dated) in order to ensure sample integrity. After the collection samples were dried in an attempt to prevent oxidation of the samples prior to analysis. See the Methods Section for more information about the collection of environmental samples.

After the samples were collected they were analyzed in the analytical laboratory located in the Earth and Planetary Sciences Department (EPS) at the University of New Mexico (UNM). Water samples were analyzed using the ICP-OES, ICP-MS and Ion Chromatography, depending on analytes of interest. Soil samples were analyzed using an acid digestion technique or water extraction. See Methods Section for more information about these analytical techniques.

The next facet of this was the modeling portion of the project. This will involve taking the analytical data and running it through two different modeling programs: PHREEQ-C and the Geochemist Work Bench. The data from the output of these two models will be used to determine the water quality via the speciation of the metals found in the water samples as the SJCPW travels through the vadose zone into the aquifer.

The final facet of this project was the data compilation and reporting. During this process, all of data that was collected from the previous two steps was analyzed to determine the water quality of the aquifer water once the SJCPW reaches it.

6.0 Methods

Each of the objectives mentioned in the section above has their own set of methods. The data collection objective used several different methods. The collected

Information included information about the Project Area, aquifer characteristics, SJCPW details, and other objectives deemed necessary to research this project.

The next step was the collection of the environmental samples. The metals samples for the aquifer waters were preserved using trace metal grade nitric acid, while the anion samples were preserved by icing (cold temperatures). All samples were refrigerated until they were analyzed. Additionally, during the sample collection process field parameters (pH, specific conductance, dissolved oxygen, temperature, and turbidity) were collected using a YSI Exo multiparameter meter. Groundwater samples were collected from the onsite monitoring wells. Additionally, five soil samples representing each of the different soil layers were collected from each of the boreholes/monitoring wells the USGS drilled during their investigation.

Each of the water samples collected (MW-3, MW-4, the Windmill Well, the Pow-Wow Well, and the Industrial Park #1 Well) were analyzed for metals using the inductively coupled plasma optical emission spectroscopy (ICP-OES), while the anions were analyzed using a ion chromatography (IC). The water samples were analyzed using an approximately 10 ml volume, without any dilution, for both of the above analytical techniques. After the water extraction the shallow zone aquifer samples were analyzed using the ICP-MS to act as a confirmatory analysis. This was performed in order to ensure that the analytes detected by the water extraction could indeed be found in the shallow zone aquifer. The samples collected from MW-3, MW-4, and the Windmill Well were analyzed in UNM's Earth and Planetary Sciences Analytical Laboratory in Albuquerque, New Mexico, while the samples collected from the Pow-Wow Well and the Industrial Park Well #1 (or IDW #1) were analyzed at the USGS National Water Quality Laboratory in Denver, Colorado.

The soil samples (approximately five per boring in MW-3, MW-4, BH-3, and BH-4) were analyzed using an acid digestion technique. This technique was performed by placing approximately 1 gram of sediment from each sample into an aqua regia solution (3ml hydrochloric acid with 1ml nitric acid). This solution was heated for

approximately two hours, which aided in the releasing of the metals bound up in the soil matrix into solution (Tessler et al, 1979). After the digestion process was completed the samples were analyzed using the ICP-OSE to determine the metal concentration released by the sediments into the aqua regia solution.

After the initial round of soil analysis was completed, data analysis was performed to determine which of the sediment samples containing metals with concentrations exceeding maximum contaminant levels (MCL). Samples that exhibited high concentrations of metals would be considered hazardous to human health. After data analysis, three different sediments samples were selected for the water extraction. These samples included two samples that exhibited elevated levels of chromium MW-3 13'-14' and BH-3 47') from the first round of analysis, in which concentrations were 103 mg/L and 91 mg/L of chromium respectively. One sample that was to be used as a background sample was analyzed, MW-3 123'-124', which was non-detect for chromium. For these samples one gram of soil was placed into a test tube with 18-mega ohm water (50ml), which was then placed into a tumbler for a various time periods. These time periods were 30 minutes, 1 hour, 2 hours, 3 hours, 4 hours, 24 hours, 25 hours, 26 hours, 47 hours, and 48 hours: at each one of the above mentioned time periods, 2 milliliters of water were removed from the test tube and diluted to ten times dilution factor by adding 8 milliliters of deionized water. These samples were then analyzed using the ICP-OES for selected elements. The above-mentioned process determined the rates at which different elements extracted from their solid phase and into solution. This round of analysis was modeled after the typical batch extraction technique to analyze the water-soluble ions found in the soil matrix (Tessler et al, 1979). The main goal of this analysis was to determine if the chromium detected during the acid extraction was the water-soluble chromium VI, which is regulated by the New Mexico Environment Department at 0.6 mg/L, and is considered to be acutely toxic by the USEPA.

After the laboratory analysis, was the modeling portion of this project. During this phase the analytical results were entered into two different modeling programs to determine the water quality of the aquifer once the SJCPW and the aquifer waters mix.

During this process piper diagrams, stiff diagrams, Phreeq-C models, and diagrams deemed appropriate for this project were created for the current groundwater, SJCPW, and the future mixed waters. This was performed using the USGS created Phreeq-C program and/or the Geochemist Workbench computer programs.

7.0 Water Results

The results of this project take three different forms. First, there are the results of the water sampling. These results are from both the shallow and deep zone aquifers located beneath the study area. See Sections 7.1, 7.1.1, 7.1.2, and 7.1.3 for more details about the results from the water analysis. Additionally, two separate rounds of soil analysis were performed. The first round of soil analysis was a whole rock (acid digestion) of 20 different samples collected from boring drilled by the USGS in November 2014. The next round of soil analysis was performed using a water extraction and then tumbling the samples for a period of 48 hours. See sections 7.2.1 and 7.2.2 for more details about the soil analysis.

7.1 Water Samples

Water samples were collected from two different sources. The shallow zone aquifer samples were collected from wells MW-3, MW-4, and the Windmill Well, which were analyzed in the University of New Mexico Earth and Planetary Sciences Analytical Laboratory in Albuquerque, New Mexico. While the deep zone aquifer samples, which were collected from the Industrial Park #1 Well and the Pow-Wow Well, were analyzed at the USGS National Water Quality Laboratory in Denver, Colorado.

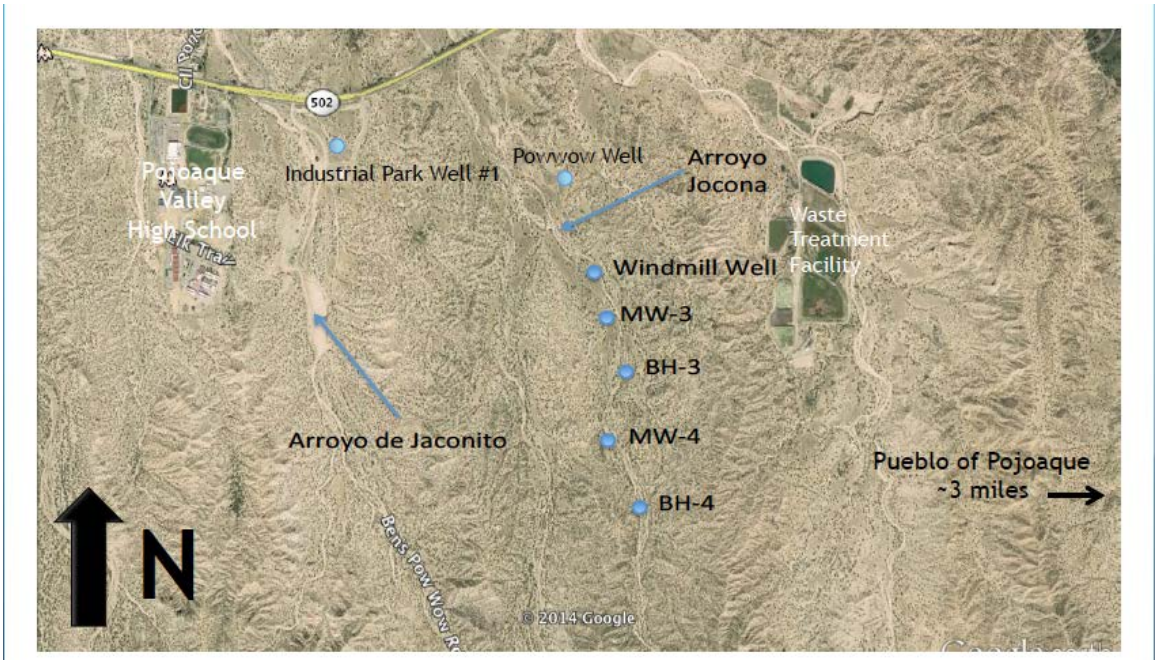


Figure 4: Locations of the wells at the Project Area

7.1.1 Shallow Zone Aquifer

The shallow zone aquifer ranges from approximately 40 to 110 feet below ground surface, or above 5,800 feet in elevation, with the direction of flow being primarily to the north. This is the aquifer system that will be the primary focus of this project. However, it should be noted that two deep zone aquifer samples were collected for comparison purposes. The hydraulic gradient of the shallow zone aquifer is from north to south, with an average slope of approximately 0.038 feet/foot or 198 feet per mile. This aquifer is primarily comprised of a sandy-clay, which exhibits a hydraulic conductivity between 10^-5 cm/sec (approximately 3.15 m/year) and 10^-3 cm/sec (approximately 315.36 m/year) (DBSA, 2014). The Daniel B. Stephens and Associates (DBS&A) Soil Analysis Laboratory performed the soil/sediment characteristics analysis for this project. However, it is believed that the average permeability is probably closer to 3 m/year, since no tritium units observed during the age dating analysis of the water in the shallow zone aquifer (USGS, 2014). This means that it is likely that no recharge has occurred in the last 60 years, and due to the small area of its recharge basin this water is moving somewhat slower than anticipated. This could have consequences for this aquifer being unable to produce enough water to be a viable drinking water aquifer.

Water	Air Pressure	Water Temp (°C)	Dissolved O2 (mg/L)	pH	SC (µS/cm)	Alkalinity (mg/L)	Turbidity (NTU)
MW-3	616.4 mmHg	15.6	4.21	7.69	474	155.7	8.84
MW-4	616.4 mmHg	13.9	7.13	7.79	374	132.4	1.44
Windmill Well	616.9 mmHg	13.4	6.6	7.65	500	143.3	37.6

Table 1: Field Parameters from the Shallow Zone Aquifer Monitoring Wells.

The shallow zone samples for the most part exhibited only a few analytes that exceeded either USEPA Drinking Water Standards or NMED Groundwater Standards. However, there were several analytes that did exceed USEPA Drinking Water Standards, only one anion exceeded standards, in one of the samples collected. Nitrates exceeded standards in the Windmill Well (see Table 1). Nitrates typically come from leaking septic tanks, or other anthropogenic sources. However, in the case of the Windmill Well it is unclear as to the source of the nitrate, since there are no known up-gradient sources for nitrate and neither of the two up-gradient wells (MW-3 and MW-4) have elevated levels of nitrate. The USEPA Drinking Water and NMED Groundwater Standard for nitrate is 10ppm (see the discussion section for possible health effects of nitrates). No other anions exceeded either the USEPA Drinking Water or the NMED Groundwater standards in the shallow zone aquifer.

Water	Br	Cl	F	Alk	NO_2	NO_3	SO_4
MW-3	0.45	21.2	1.10	155.7	ND	3.69	66.0
MW-4	0.37	14.4	1.01	132.4	ND	6.21	33.0
Windmill Well	0.01	15.1	1.13	143.3	ND	15.2	70.6
EPA Drinking Water Standards	--	250	4	--	1	10	250*
NMED GW Standards	--	250	1.6	--	--	10	250

Table 2: Anions in the Shallow Zone Aquifer. Values in Red exceed USEPA Drinking Water Standards. All values are shown in mg/L.

Metals (cations) in the shallow zone aquifer exhibited a similar trend to that of the anions, meaning that most of the constituents were below the USEPA Drinking Water Standards and the NMED Groundwater Standards. However, there were two analytes that exceeded USEPA Drinking Water Standards in all of the wells sampled. These

analytes included both aluminum and lead (see the discussion section to for health effects of lead and aluminum). It is hypothesized that the elevated aluminum concentrations is from the dissolution of aluminum from clays, either illite or smectite based on the USGS XRD analysis, which these clays are believed to be the primary constituents of the shallow zone aquifer. However, lead is primary considered to be an anthropogenic so it is unclear as to the source of the elevated lead concentrations in the shallow zone aquifer. No other analytes exceeded either USEPA Drinking Water Standards or NMED Groundwater Standards in the shallow zone aquifer. See Table 2 for a listing of selected metals detected in the shallow zone aquifer.

Water	Al	As	Ba	Cd	Cr	Cu	Fe	Pb	Mn	U	Zn
MW-3	55	14	97	<20	11	29	<1	27	<6	NA	27
MW-4	55	14	70	<20	12	30	<1	26	<6	NA	<17
Windmill Well	51	12	82	<20	9	30	4	26	28	NA	102
EPA Drinking Water Standards	50	10	2,000	500	100	1,300	300	15	50	30	5,000
NMED GW Standards	5,000	100	1,000	10	50	1,000	1,000	50	200	--	10,000

Table 3: Selected metals from the shallow zone aquifer. Values in Red exceed USEPA Drinking Water Standards. All values are shown in µg/L.

7.1.2 Deep Zone Aquifer

The deep zone aquifer is found at a depth of approximately 150 feet below ground surface at the subject site, or below 5,800 feet in elevation, with the flow direction primarily being from east to west (USGS, 2014). The recharge zone for these waters is in the Santa Fe Mountains located approximately 20 miles to the east of the study site. Additionally, this aquifer tends to be the primary aquifer for drinking water for the communities located to the north and east of the study site. Unfortunately, this aquifer is characterized by having several constituents that exceed the USEPA Drinking Water Standard. These analytes are typically uranium, arsenic, and fluoride (Wolfe, 2014)

Water	Air Pressure	Water Temp (°C)	Dissolved O2 (mg/L)	pH	SC (µS/cm)	Alkalinity (mg/L)	Turbidity (NTU)
IPW #1	627 mmHg	22.3	1.2	8.64	960	375.5	--
Pow-Wow Well	618 mmHg	15.5	1.6	9.69	357	116	1.5

Table 4: Field Parameters from the monitoring wells in the Deep Zone Aquifer.

Water	Br	Cl	F	Alk	NO_2	NO_3	SO_4
Industrial Park Well #1	0.16	10.4	**6.2**	375.5	0.0	0.0	44.1
Pow-Wow Well	0.16	11.3	1.3	116.0	0.02	1.0	42.8
EPA Drinking Water Standards	--	250	4	--	1	10	250
NMED GW Standards	--	250	1.6	--	--	10	250

Table 5: List of Anions detected in in deep zone aquifer. Vales in **Green** exceed both USEPA Drinking water and NMED Groundwater Standards. All values are shown in mg/L

Much like the historical results, the results of this study exhibited a similar trend in the data. Previous studies have shown uranium as high as 567 µg/L in the deep zone aquifer (McLemore et al, 2011). With the two uranium-mining districts located near the study sites, elevated uranium values wouldn't be unexpected. The fluoride is hypothesized to be from ash beds that are located within the Tesuque Formation. With the lack of calcium in these waters, there isn't any mechanism for the controlling fluoride concentrations in these waters (Table 4). It can be observed in Figure 5 that the Industrial Park Well #1 that most of the cation concentrations in this well is sodium, while the calcium concentrations are very low allowing for the fluoride to concentrate in this well. It isn't unusual for arsenic to be associated with volcanic rocks, and with the Jemez Mountains located approximately 10 miles to the west of the study site this could account for any possible arsenic found at the study site. For this study the analytical results from the Industrial Park Well #1 had elevated concentrations of both arsenic (27.6 µg/L) and fluoride (6.2 µg/L) as compared to USEPA Drinking Water Standards. See the Discussion Section to see potential health effects of these analytes. While uranium didn't exceed the USEPA Drinking Water Standard (30 µg/L) in either of the wells sampled, the sample collected from the Pow-Wow Well had the highest detection with 24 µg/L, which is below the USEPA Drinking Water Standard. No other analytes exceeded either the USEPA Drinking Water Standards or the NMED Groundwater Standards in the deep zone aquifer. See Table 4 for selected metals detected in the deep zone aquifer.

Water	Al	As	Ba	Cd	Cr	Cu	Fe	Pb	Mn	U	Zn
Industrial Park Well #1	10.4	27.6	2.9	<0.03	<0.03	3.72	49	0.6	6.5	0.2	<2.0
Pow-Wow Well	14.8	9.6	2.5	<0.03	1.67	<0.8	12.4	0.1	<0.04	24	8.5
EPA Drinking Water Standards	**50**	**10**	**2,000**	**500**	**100**	**1,300**	**300**	**15**	**50**	**30**	**5,000**
NMED GW Standards	**5,000**	**100**	**1,000**	**10**	**50**	**1,000**	**1,000**	**50**	**200**	**--**	**10,000**

Table 6: Selected list of metals found in the Deep Zone Aquifer. Values in Red exceed the USEPA Drinking Water Standards. All values are shown in µg/L.

7.1.3 Comparison of Waters

For this project the deep zone aquifer was not the primary focus, since it is not anticipated for water from this project to come into contact with water from the deep zone aquifer. However, two samples were collected for comparison purposes. These samples were collected from the Pow-Wow and the Industrial Park Well #1. See Figure 5 for a comparison between Shallow Zone and Deep Zone aquifer waters using a Piper Diagram, while Figure 6 compares the same waters but uses a series of Stiff Diagrams. The two surface water bodies used in these diagrams are the Rio Grande at Otowi and Tesuque Creek. Both samples were collected and analyzed by the USGS. Both Piper and Stiff diagrams visually compare the waters, with the major difference being the platform used to compare the waters and how the concentrations are compared. Both compare the waters visually using the concentrations of the major cations (calcium, magnesium, potassium, and sodium) and major anions (chloride, sulfate, carbonate, and bicarbonate). For a Piper Diagram the concentrations used are percentages, while a Stiff Diagram uses milliequivalents per liter. Milliequivalents per liter (meq/L) are an expression of the concentration of the compound divided by the molecular weight, which is then divided by the charge of the compound. In the case of the calcium concentration (which has a charge of +2) in MW-3, which was 48.46 mg/L, the meq/L would be 48.46/(40/2) which equals 2.42 meq/L.

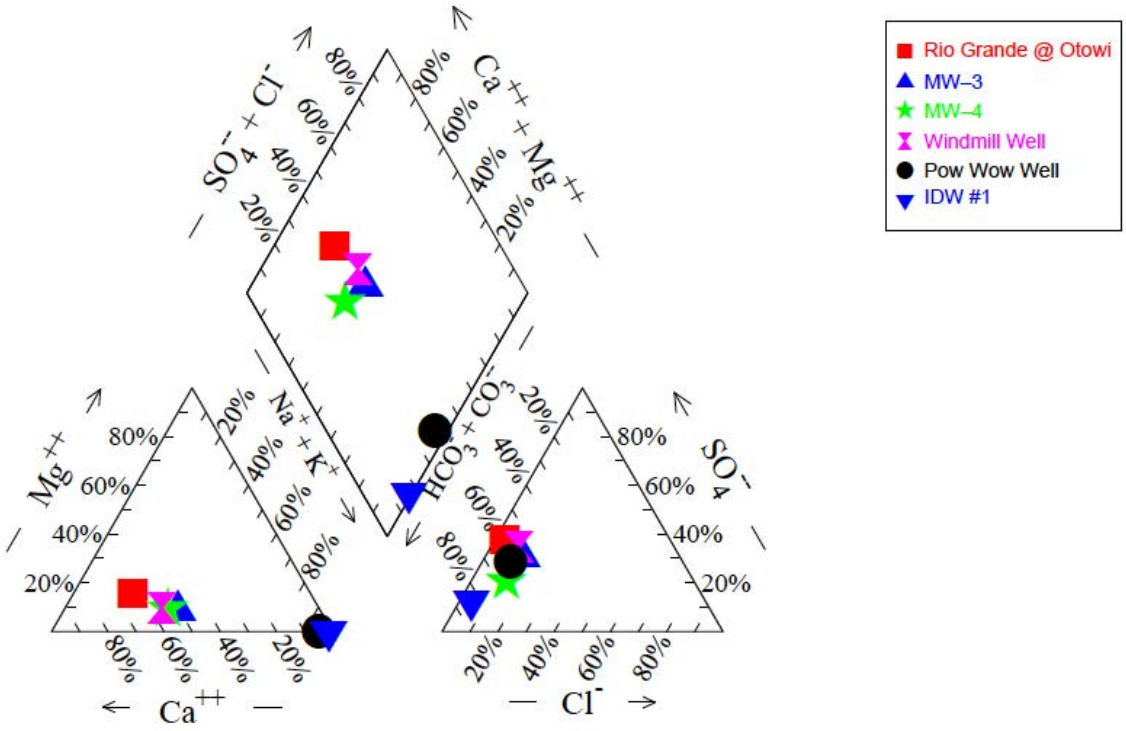


Figure 5: Piper diagram of water located in the Study Area

Figure 5 illustrates that the waters from similar zones tended to group together in the Piper Diagram. This shows that the grouped waters have similar characteristics, and flow paths through their various formations. In the case of the deep zone aquifer the waters from the Pow-Wow and Industrial Park Well #1 Wells the ratio of constituents are similar. However, the analytes in the Industrial Park Well #1 are much more concentrated. Between the concentrated constituents and being located down gradient from the Pow-Wow Well lead us to believe that the water found in the Industrial Park Well #1 is older than the water found in the Pow-Wow Well.

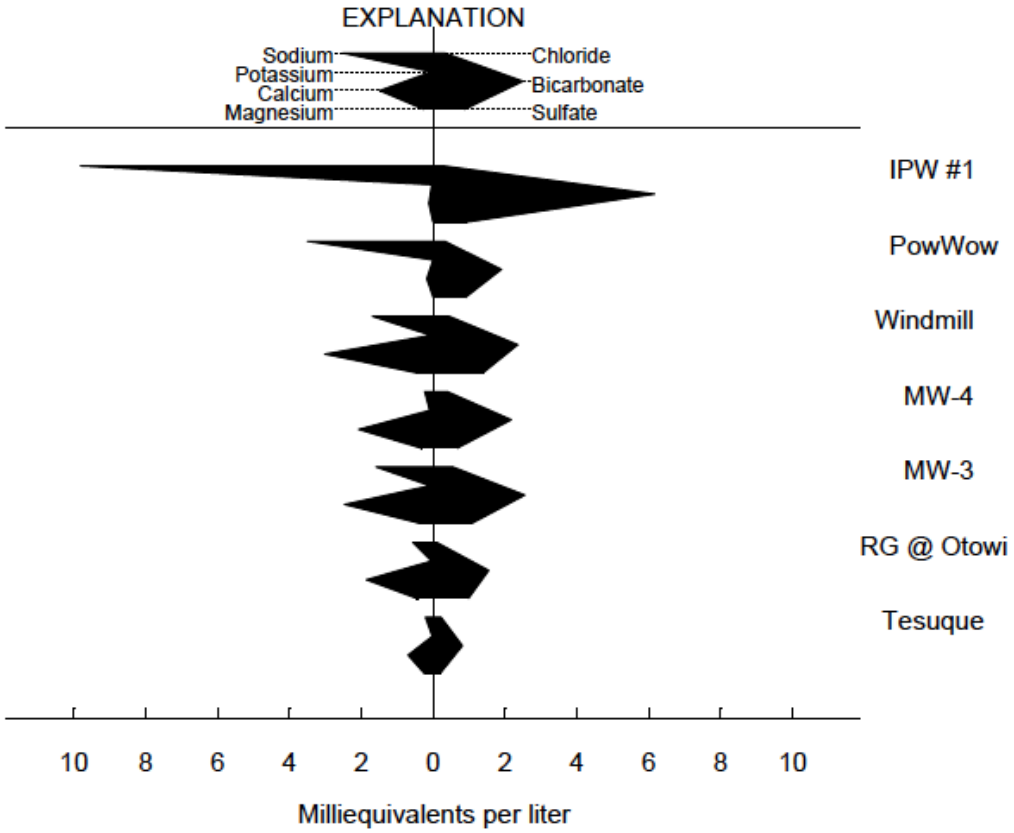


Figure 6: Stiff Diagrams of waters located in the Study Area.

When compared using Piper and Stiff diagrams a visual difference in the waters can be observed. With the Stiff Diagrams the difference in the zones can be observed in the shape and the size of the symbols for each of the waters. For the Stiff Diagrams the symbols from the same zone are similar in shape, and in the case of the shallow zone the symbols are approximately the same size. However, Stiff and Piper diagrams have the disadvantage of only comparing the major ion/ constituents to each other, while the minor constituents don't get compared. For this study minor constituents in each of the water samples were compared by graphing them in Microsoft Excel®, and them comparing them to the USEPA Drinking Water and NMED Groundwater Standards. See Figure 7 for a graph of minor constituents in the waters found in and near the study area.

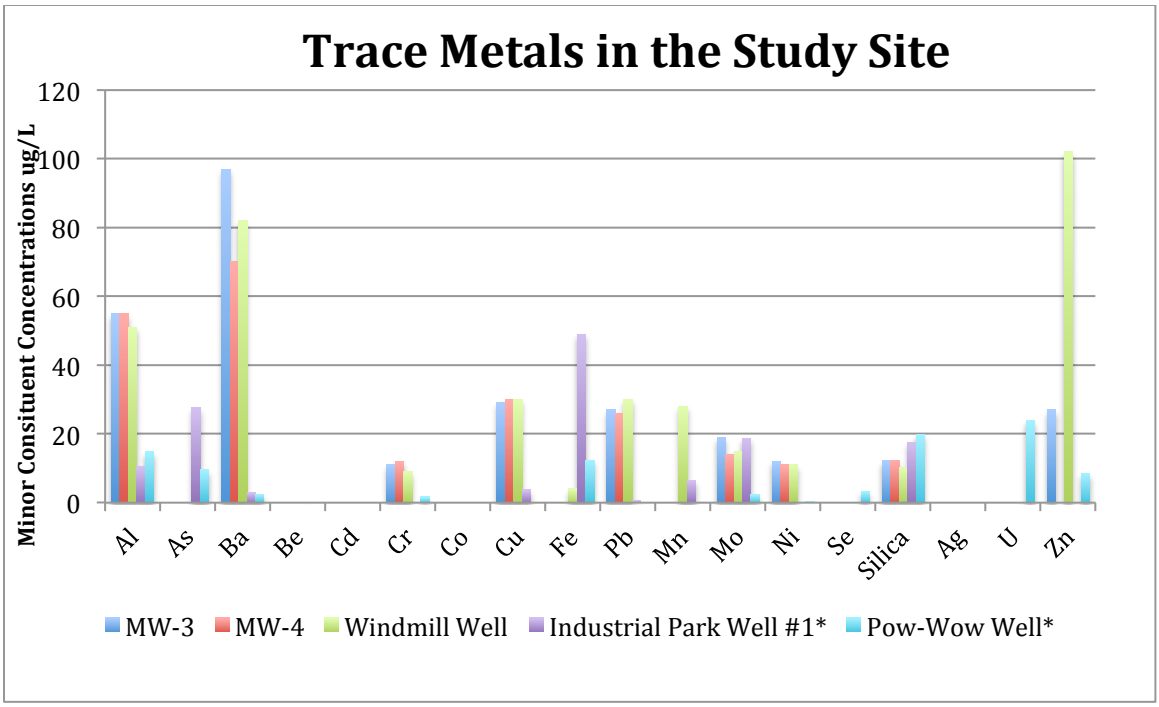


Figure 7: Graph of minor constituents from the waters found in and near the study site. All constituent concentrations are shown in µg/L. Deep zone wells have asterisk.

Figure 7 shows that the concentration of most of the minor constituents in the shallow zone aquifer are more concentrated than they are in the deep zone aquifer, with the notable exception of arsenic and uranium where these constituents are found at non-detect levels in the shallow zone aquifer. It should be noted that most of the concentrations of these constituents are below the USEPA Drinking Water Standards. As previously stated, there are a few exceptions to the above statement. Aluminum and lead exceed the USEPA Drinking Water Standards in MW-3, MW-4, and the Windmill Well, which are all shallow zone wells. Arsenic and fluoride exceed the USEPA Drinking Water Standard in the Industrial Park Well #1 a deep zone well. See the discussion section for possible treatment options for the above-mentioned exceedances.

7.2 Soil Results

The soil samples analyzed for this project were collected from soil borings that the USGS drilled in November 2014. Two of the soil borings that were drilled by the USGS were completed as monitoring wells MW-3 and MW-4. Sediments beneath the

study site ranged from coarse-grained gravelly sands, located near the surface, to fine-grained sandy-clays, which are located deeper in the aquifer portion of the boreholes. The boring logs from the drilling of these wells are attached in Appendix 1. Two analytical techniques that were used to analyze the soil samples included an acid extraction and a water extraction. All of the soil analyses performed for this project were analyzed in the UNM Earth and Planetary Sciences Analytical Chemistry Laboratory. See the Sections 7.2.1 and 7.2.2 below for specific details and analytical results from the soil analysis from the study site.

7.2.1 Acid Extraction

The acid digestion portion used an aqua regia solution (3 ml hydrochloric acid and 1 ml nitric acid) to extract metals from the soil samples, after which the samples were analyzed with the ICP-OES. This analytical method was performed to determine whether or not any metals were found at elevated concentrations in any of the soil samples. This would provide an indication of what soil samples should be analyzed using the batch extraction. All of the soil samples collected by the USGS (20 different samples) were analyzed using this technique.

After this analysis was performed the analytical results were compared to NMED Residential Soil Screening Standards, which is more conservative than either the commercial or industrial soil screening levels. Additionally, the analytical results were used to determine which soil samples would be used in the water extraction.

It was hypothesized that the uranium and arsenic would exceed the NMED Residential soil screening levels. However, this was not to be the case. In the UNM Acid Extraction both the arsenic and uranium levels were found to be non-detect. However, in the USGS XRF data both arsenic and uranium were found at detection levels. It should be noted that the ICP-OES doesn't have good low-level resolution for uranium, which could have resulted in the non-detect reading. One arsenic sample was found to exceed the NMED Residential Soil Screening level (3.9 mg/kg) in sample BH-4 28'-29' with a detection of 4.7 mg/kg. For uranium, the maximum detection is 37 mg/kg

in the sample collected from MW-3 42'-43'. This detection is well below the NMED Residential Soil Screening level of 235 mg/kg. The original hypothesis, exceedances of arsenic and uranium, was determined to not be an issue in these sediments; however, another potential issue that was discovered which is potentially chromium.

Chromium is the only metal regulated by the NMED depending on its valence state. Chromium-III (3) is considered to be less toxic and is regulated by the NMED Residential Soil Screening Level at 1,200 mg/kg, while Chromium-VI (6) is considered to be highly toxic and the NMED soil screening level is 2.97 mg/kg. In addition to being highly toxic Chromium-VI is more water-soluble than Chromium-III. This could pose an issue for human health if consumed at a high enough concentration in the drinking water. However, for this aspect of the project, the speciation of the chromium found in the sediments was not established.

The total chromium concentrations found in the boreholes ranged between 12 mg/kg in BH-4 56'-57' to 103 mg/kg in MW-3 13'-14'. Both of these concentrations are above the NMED Residential Soil Screening Level for Chromium-VI, while below the level for Chromium-IV. Although determining the source of the chromium in these sediments in not within the scope of this project, it is hypothesized that the chromium is volcanic in origin. This hypothesis originated in the fact that in all of the boreholes there were two distinct chromium detections where the layers approximately lined up with each other. MW-3 was the exception to this rule, with only having one layer that exhibited chromium detection.

Various other metals were detected in the boreholes beneath the project site during the acid extraction portion of this project. For this paper, only the metals that were detected will be listed. These non-detect metals for this portion of the analytical process included arsenic, beryllium, cadmium, cobalt, lead, molybdenum, selenium, and vanadium. Even though other metals were detected during this portion of the analytical process, none of their detection levels exceeded the NMED Residential Soil Screening

Levels. See Table 5 for selected metals that were detected during the acid digestion analysis for this project.

Sample	Al	B	Ba	Cr	Cu	Fe	Li	Mn	Ni	Sr
MW-3 13-14	2,500	29	205	**103**	38	7,300	45	125	5	69
MW-3 42-43	9,700	47	202	<0.5	51	12,500	30	882	<3.3	259
MW-3 93-94	1,500	16	44	<0.5	16	2,700	74	17	<3.3	18
MW-3 114-115	4,900	32	510	<0.5	38	8,200	72	125	<3.3	280
MW-3 123-124	6,600	41	198	<0.5	40	11,500	79	225	<3.3	104
BH-3 12-13	1,100	20	162	<0.5	35	3,700	71	10	<3.3	12
BH-3 36-37	5,400	30	261	<0.6	38	7,500	71	94	<2.5	158
BH-3 54-55	4,600	30	182	**21.1**	38	7,300	79	141	<2.7	95
BH-3 74-75	7,500	45	207	<0.3	42	11,300	71	231	<2.5	118
BH-3 86-87	4,400	47	245	**38.1**	39	9,200	78	112	<3.0	159
BH-4 19-20	1,500	24	162	<0.5	35	5,700	72	19	<3.1	18
BH-4 28-29	6,000	40	296	<0.5	44	8,000	73	48	<2.7	76
BH-4 30-31	1,800	25	176	**52**	40	5,400	72	ND	<2.9	16
BH-4 50-51	2,400	34	501	<0.5	36	5,100	66	71	<2.5	28
BH-4 56-57	1,700	22	148	**12**	36	4,800	31	45	<2.5	25
MW-4 12-13	1,100	20	162	<0.5	35	3,700	71	10	<3.1	12
MW-4 36-37	5,400	30	261	<0.5	38	7,500	71	94	<2.5	158
MW-4 54-55	4,600	30	182	**21.1**	38	7,300	79	141	<2.6	95
MW-4 74-75	7,500	45	207	<0.5	42	11,300	71	231	<2.9	118
MW-4 86-87	4,400	47	245	**38.1**	39	9,200	78	112	<3.0	159
NMED SSL	**78,000**	**15,600**	**15,600**	**2.97**	**3,130**	**54,800**	**N/A**	**1,860**	**1,560**	**46,900**

Table 7: Selected metals from the acid extraction analysis. Values in **Red** exceed NMED Residential Soil Screening Levels. All values are shown in mg/kg.

7.2.2 Water Extraction

The water extraction was designed to determine which metals would come out of their solid phase to imitate recharged water reacting with sediments. This was modeled after several studies in which 18-mega ohm water was used to extract the water extractable constituents within the soil matrix (Tessler et al, 1979). Since only SJCPW is going to be moving through the soil matrix, only the water portion of the batch extraction process was performed. 18-mega ohm water was used instead of SJCPW so it was be easily observable as to which constituents were leaching out of the soil matrix.

Three soil samples were selected: MW-3 13'-14' and BH-3 47' were selected because previous results indicated that they had elevated chromium concentrations. MW-3 123-124' had a low chromium concentration and was included as a control sample. Additionally, three of each sample was run as replicates in order to evaluate quality control. In addition each of these layers represented a different lithologies from within the boreholes. MW-3 13'-14' consists primarily of a fine grained sand, BH-3 47' consists primarily of a fine grained sandy-clay, and MW-3 123' consists primarily of a fine grained clay.

In order to perform this round of analysis approximately 2 grams of soil was placed into 50 milliliters of 18-mega ohm water, after which the samples were placed into a tumbler and were then rotated for a total of 48 hours, during which samples were collected at various intervals throughout the 48 hour period. The sampling intervals were 30 minutes, 1 hour, 2 hours, 3 hours, 24 hours, 25 hours, 26 hours, 27 hours, 47 hours, and 48 hours. The samples were diluted 10x, and analyzed using the ICP-OES.

This analysis was designed to determine whether or not chromium exceeds USEPA Drinking Water Standards. The USEPA Drinking Water Standard for chromium is 100 μg/L, which means that any higher concentrations would result in actions having to be taken in order to protect human health. It was found that none of the samples analyzed had elevated chromium concentrations. The highest chromium concentration observed is 8.90 μg/L, in sample MW-3 13'-14' #1 at 47 hours, which is well below the USEPA Drinking Water Standard. This means that most of the chromium observed in the layers beneath the study area should consist of the lower toxicity and less water soluble Chromium-III, and shouldn't be an issue for human consumption. Even though chromium isn't considered to be an issue for this project, there are other analytes that were detected during the analytical process that weren't detected at elevated levels during the other previous analysis. During the water extraction only zinc was found to be at non-detect levels.

Several constituents were analyzed were found to be at levels exceeding the USEPA Drinking Water Standards. These constituents include aluminum, arsenic, beryllium, and iron which all exceeded standards in at least one of the samples analyzed. The USEPA Drinking Water Standards for these analytes are 50µg/L, 10µg/L, 4µg/L, and 300µg/L respectively. Each of the above mentioned analytes are to be discussed separately in the following paragraphs. During the water extraction analysis anions were not analyzed for, due to the lack of sample volume. See Tables 6 through 8 for selected constituents from the water extraction. The selected constituents in these tables are only constituents that have USEPA Drinking Water Standards, and also that the values in the table are averaged between the values from the three replicates, since the values between samples tended to be relatively close.

Time (hrs)	Al	As	Ba	Be	Cd	Cr	Cu	Fe	Pb	Mn	Se
0.5	245.6	44.1	43.8	82.9	7.0	7.8	59.3	98.7	39.2	4.7	38.6
1	261.1	42.8	43.7	82.9	7.0	7.9	59.3	108.5	40.3	3.0	35.7
2	260.7	43.9	43.7	82.9	7.0	7.7	59.2	109.0	38.1	3.4	36.0
3	244.2	43.9	43.8	82.9	6.9	7.9	59.0	98.3	37.7	3.2	29.7
24	297.2	44.0	44.0	83.0	7.0	8.1	58.9	132.0	40.3	3.9	31.4
25	127.2	44.7	34.1	83.3	7.2	7.7	59.7	24.3	40.5	5.6	41.3
26	229.1	45.9	34.4	83.2	7.1	7.8	59.5	89.4	39.9	6.1	36.5
27	126.5	43.1	43.6	83.0	7.0	7.6	59.4	23.9	39.6	3.9	34.3
47	342.7	45.7	44.3	82.9	7.0	8.0	59.2	161.1	40.6	5.5	30.7
48	380.6	41.9	44.5	82.9	7.0	7.8	59.3	183.9	40.0	5.9	34.7
USEPA DWS	**50***	**10**	**2,000**	**4**	**500**	**100**	**1,300**	**300***	**15**	**50**	**50**

Table 8: Averaged values from BH-3 47' from the water extraction. All values shown are in µg/L. Asterisked values are secondary USEPA Drinking Water Standards

Time (hrs)	Al	As	Ba	Be	Cd	Cr	Cu	Fe	Pb	Mn	Se
0.5	219.7	42.9	66.1	82.6	6.8	7.6	59.0	76.1	38.1	4.2	31.4
1	264.4	41.8	64.0	82.6	7.0	7.9	59.0	107.1	38.5	3.5	31.0
2	430.3	43.7	64.5	82.5	6.9	8.0	59.0	201.7	37.2	4.1	32.8
3	432.2	46.1	64.8	82.8	7.1	7.9	59.0	203.7	38.3	4.6	30.7
24	659.9	43.6	66.2	82.4	6.9	8.4	58.5	349.5	41.7	6.5	33.5
25	371.6	44.5	64.5	82.6	7.0	7.7	59.1	172.3	39.7	5.0	32.1
26	194.8	45.0	63.3	82.5	7.0	7.6	59.0	64.8	38.5	5.1	34.2
27	497.4	44.6	67.8	82.5	7.0	7.8	59.1	250.4	40.3	10.6	32.2
47	899.4	40.4	72.8	82.5	6.9	8.6	58.6	496.0	41.2	10.7	28.2
48	1010.8	42.8	76.1	82.5	7.0	8.3	59.4	557.0	41.3	12.2	26.4
USEPA DWS	**50**	**10**	**2000**	**4**	**500**	**100**	**1300**	**300**	**15**	**50**	**50**

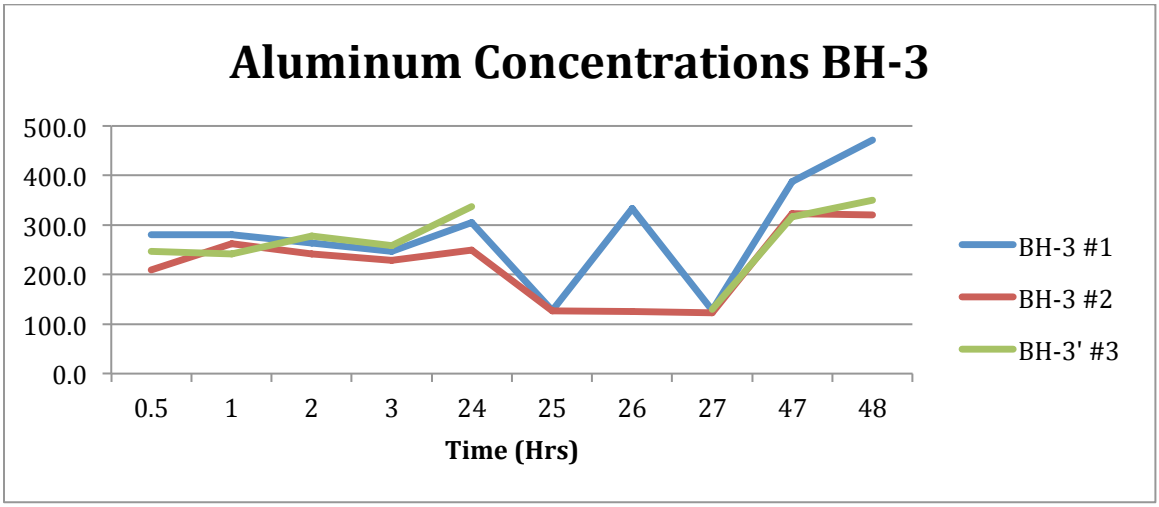
Table 9: Averaged values from MW-3 13'-14' from the water extraction. All values shown are in µg/L. Asterisked values are secondary USEPA Drinking Water Standards

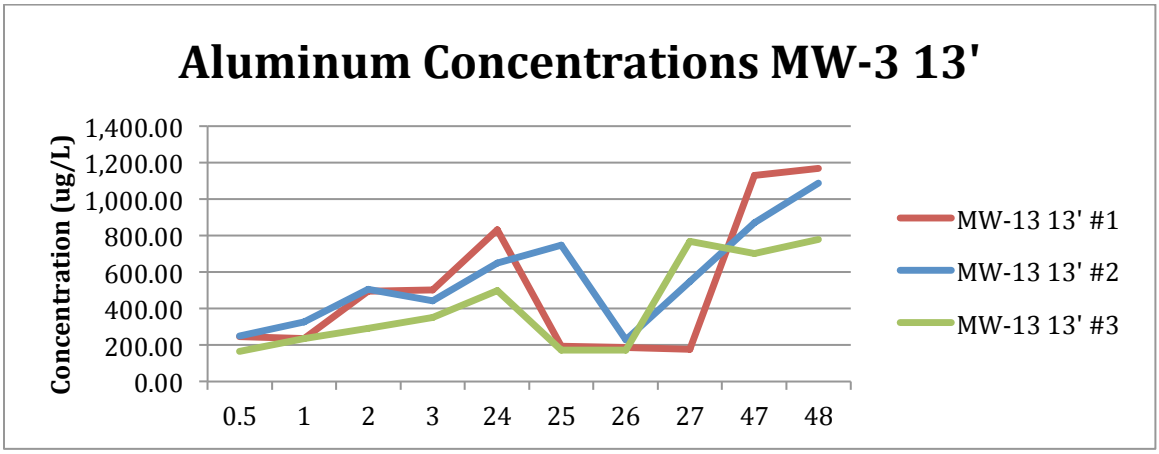
Time (hrs)	Al	As	Ba	Be	Cd	Cr	Cu	Fe	Pb	Mn	Se
0.5	195.8	41.2	62.3	82.7	6.9	7.6	59.2	70.3	39.0	4.4	37.0
1	253.9	42.5	63.2	82.7	6.9	7.9	59.2	102.6	39.9	3.7	32.7
2	244.9	41.2	62.4	82.8	7.0	7.9	59.1	103.3	40.3	3.4	31.0
3	268.5	44.3	62.4	82.7	6.9	7.9	58.8	119.4	39.6	3.6	30.7
24	488.0	41.7	62.9	82.6	6.9	8.1	58.7	262.0	39.7	5.1	30.3
25	136.3	42.2	62.0	82.8	6.9	7.6	59.3	31.7	40.0	7.1	34.1
26	276.2	44.8	64.1	82.8	7.1	7.7	59.2	121.3	40.7	7.1	34.6
27	355.0	43.5	63.1	82.7	7.0	7.8	59.0	174.7	40.0	6.8	32.2
47	690.3	41.8	63.3	82.7	7.0	8.1	58.9	392.5	39.5	6.7	26.7
48	748.1	42.8	64.4	83.2	7.3	8.2	42.6	430.2	40.7	12.2	34.0
USEPA DWS	**50**	**10**	**2000**	**4**	**500**	**100**	**1300**	**300**	**15**	**50**	**50**

Table 10: Averaged values from MW-3 123'-124' from the water extraction. All values shown are in µg/L. Asterisked values are secondary USEPA Drinking Water Standards

Aluminum is the first constituent to be discussed in this section. Aluminum tends to be mobile primarily at lower pH's. With the primary constituent of the aquifer beneath the study site being clay, it's not surprising that aluminum would exceed the USEPA Secondary Drinking Water Standard of 50 µg/L (USEPA, 2015). USEPA Secondary Drinking Water Standards are standards that don't typically effect human health, but instead affect the aesthetic qualities of the water. Secondary standards tend to be suggestions. In fact all of the samples analyzed during the water extraction exceeded

USEPA Secondary Drinking Water Standards. Aluminum concentrations ranged from 133 µg/L (MW-3 123'-124' #3) up to 1,167 µg/L (MW-3 13'-14' #2). Aluminum is considered to be hazardous to both humans and aquatic organisms in high enough concentrations. See the discussion section for more information about how aluminum can negatively affect human health. Figure 4 shows the aluminum concentrations in all of the different samples collected, including the replicate samples.





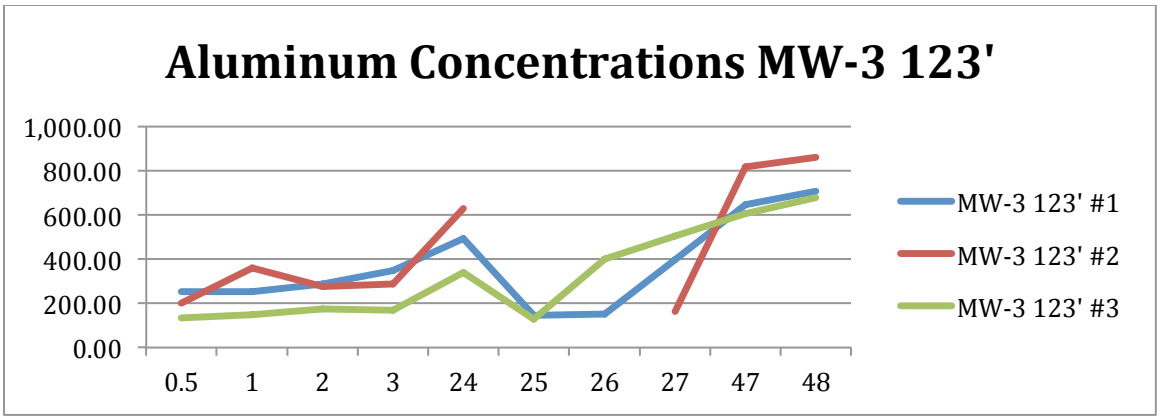
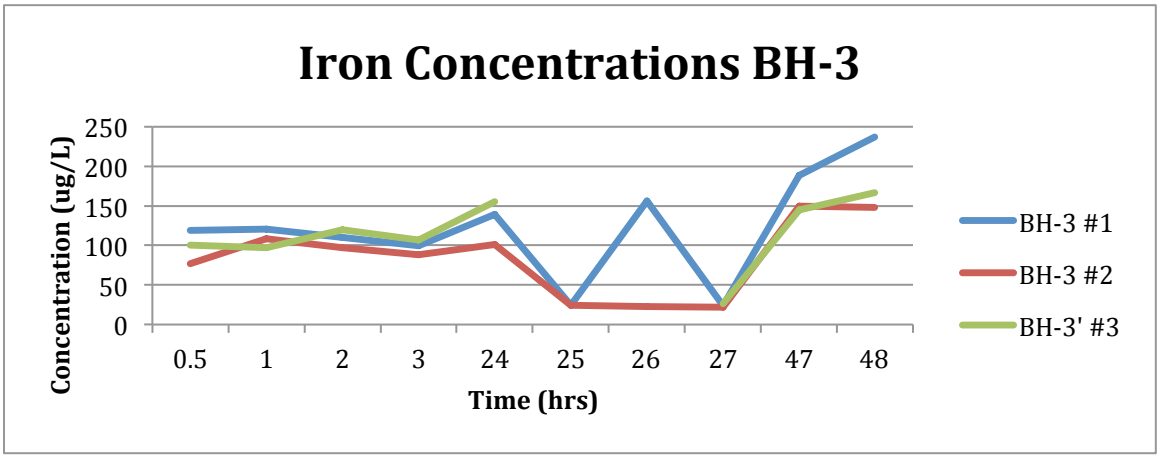


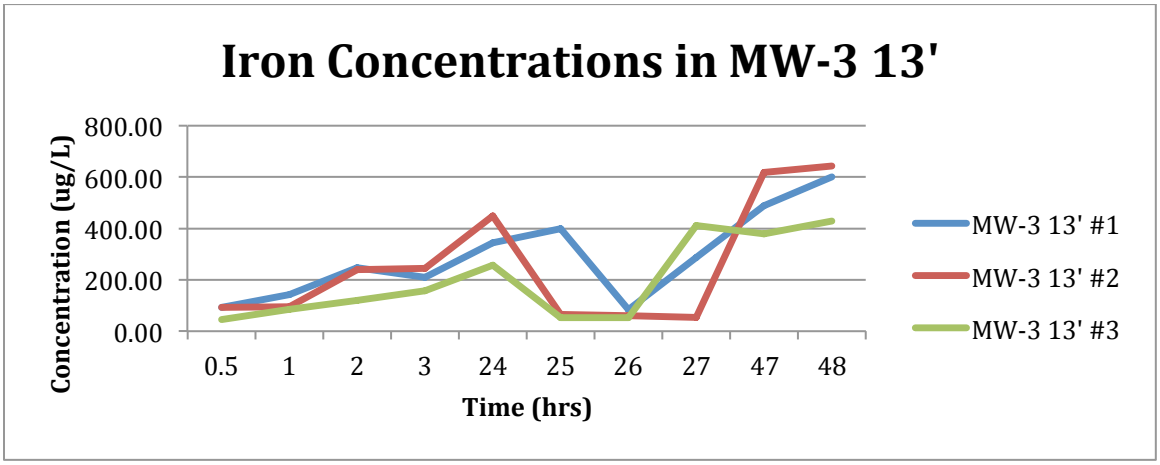
Figure 8: Concentrations of aluminum from the water extraction. All concentrations are shown in µg/L.

As it can be observed the aluminum concentrations in all of the samples decreases at approximately 24 hours. These concentrations remained at a lower level than was anticipated, and remained low until sometime between 27 hours and 47 hours. After the initial earlier time period, the aluminum concentrations increased to the highest concentrations observed during the sampling time period. The possible explanation for the decreasing of aluminum concentrations is that some of the aluminum was precipitated as a clay mineral. While after 27 hours the aluminum concentrations increased due to the aluminum re-dissolving. In addition to the aluminum concentrations, calcium, iron, magnesium, and silica exhibited the same trend around the same time period. All of the above-mentioned elements are constituents of various clay minerals. However, no satisfactory explanation was hypothesized for this phenomenon, as it was not the focus of this study and shouldn't have any negative effects on water quality.

Iron is the next element to be discussed. Much like aluminum, iron is another constituent of clay minerals, primarily illite and smectite, and with clays being a major constituent of the aquifer beneath the study site its not surprising that iron would exceed USEPA Secondary Drinking Water Standard of 300 µg/L (USEPA Contaminants, 2015). Additionally, oxidized iron could be observed in the soil samples before they were processed for analysis. Unlike aluminum, iron doesn't exceed the USEPA Drinking Water Standards for the entirety of the sampling event. In fact none of the samples analyzed from BH-3 exceeded the USEPA Drinking Water Standards. The only exceedances of USEPA Drinking Water Standards in the samples collected from both

MW-3 13'-14' and MW-3 123'-124' were the samples collected at 47 hours and 48 hours, and approximately half of the samples analyzed at the 24-hour collection period exceeded the USEPA Drinking Water Standards. See the discussion section for possible health effects of iron on human health. Figure 9 shows the iron concentrations in all of the different samples collected, including the replicate samples.





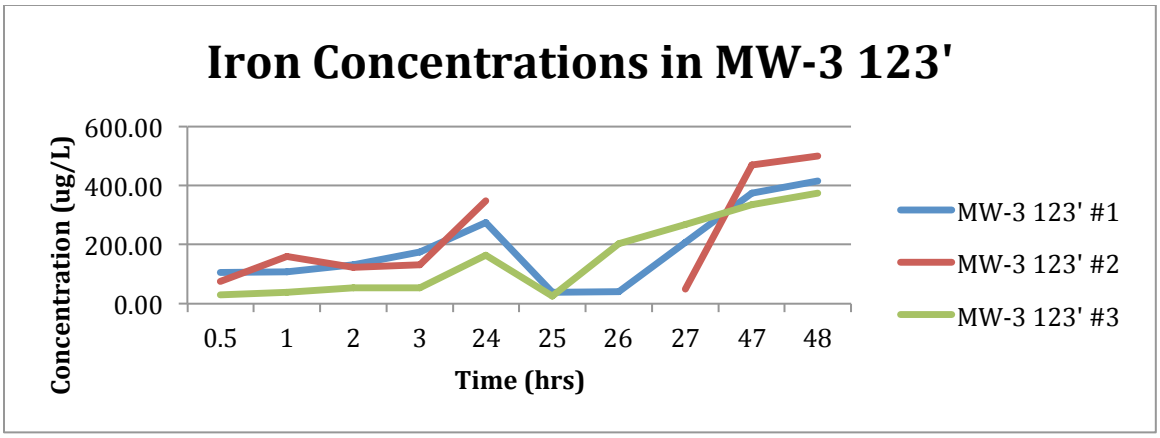
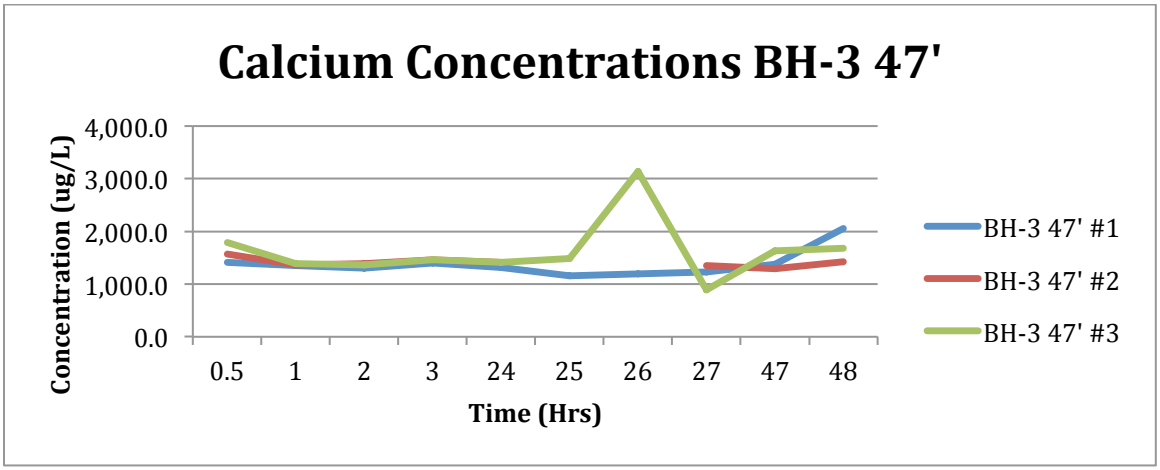


Figure 9: Graphs of iron concentrations in the water extractions. All concentrations are shown in ug/L.

It should be noted that the graphs for both iron and aluminum have nearly an identical shape. The graphs for magnesium and silica, which will be shown as Figures 11 and 12, have a nearly identical shape. It is hypothesized that that one or more of these elements reached its saturation point, and as it comes out of solution it's causing other elements to come out of solution with it to form clays. The dissolution of these elements could result in such issues as clogging within the sediments, which would negatively impact the waters ability to recharge efficiently. However, when it comes to a water quality stand point these clays shouldn't be an issue. See Figures 10, 11, and 12 for graphs of the concentrations of calcium, magnesium, and silica.



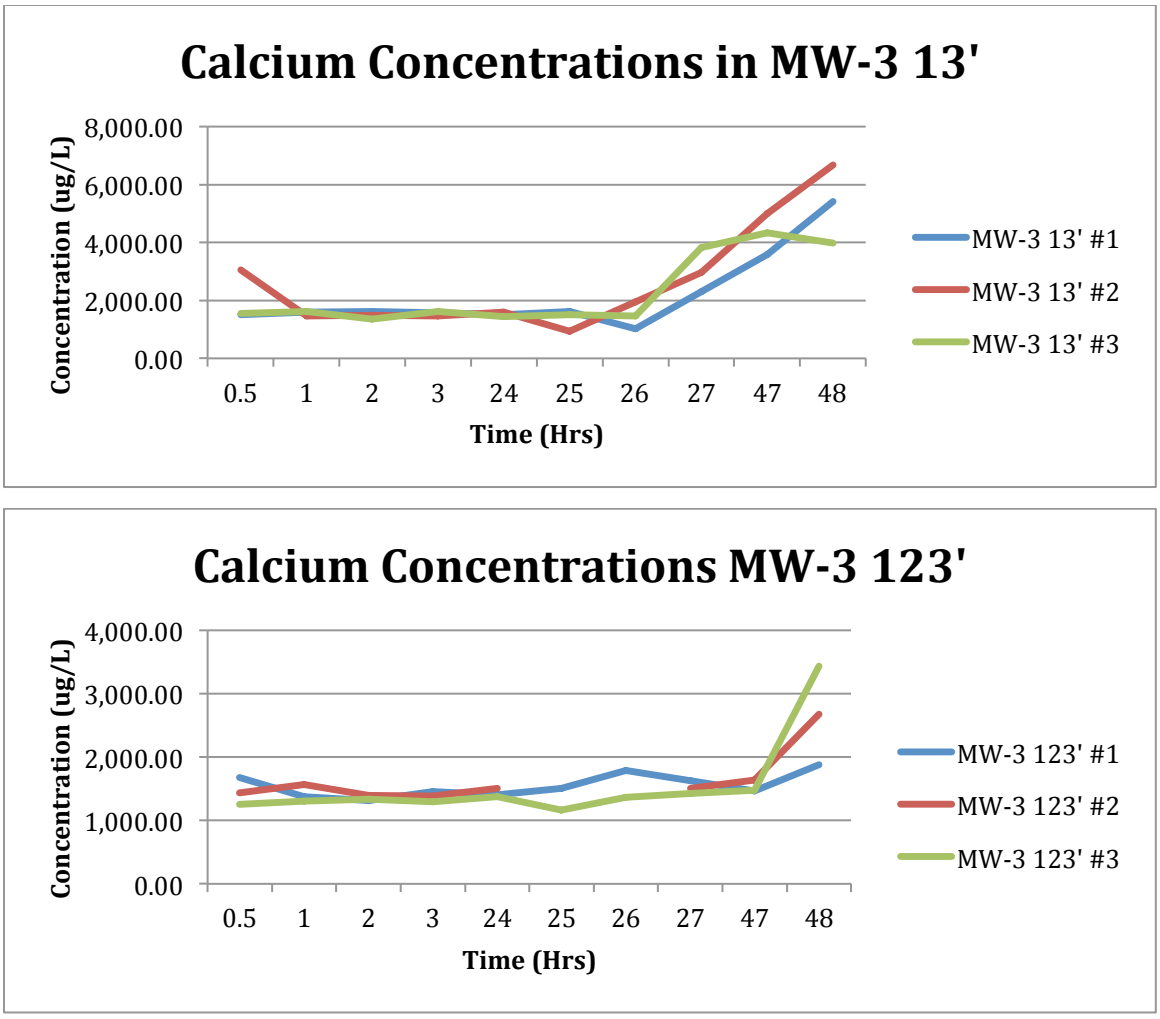
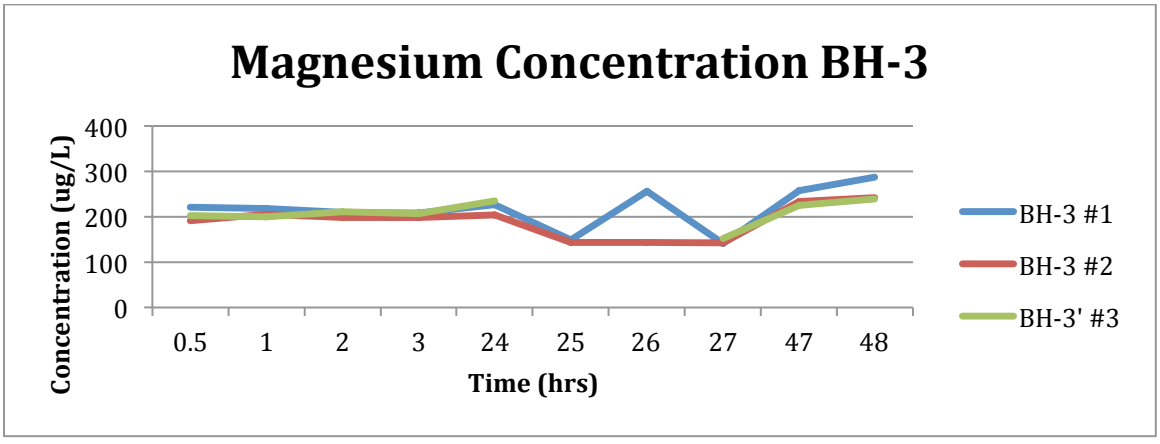
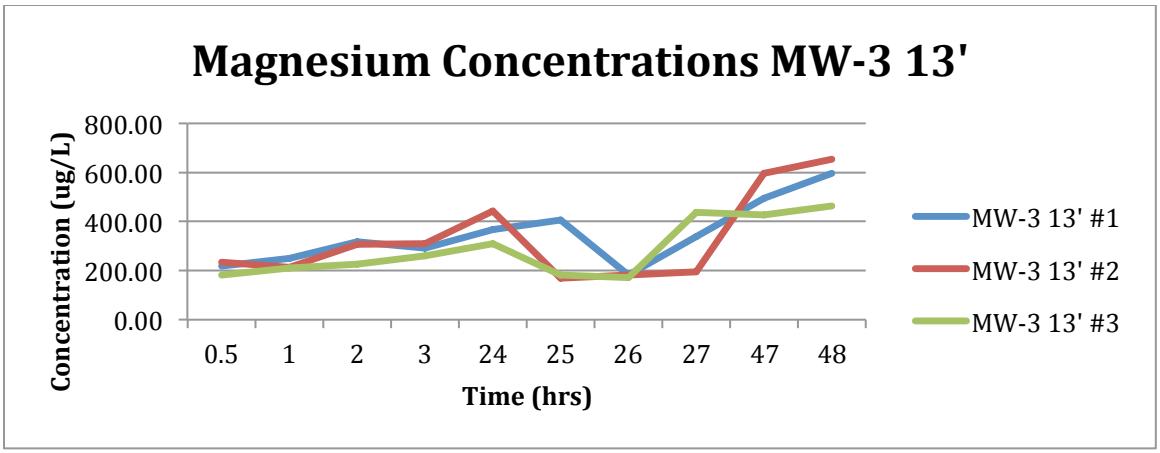


Figure 10: Calcium concentrations from water extraction, concentrations shown in ug/L.





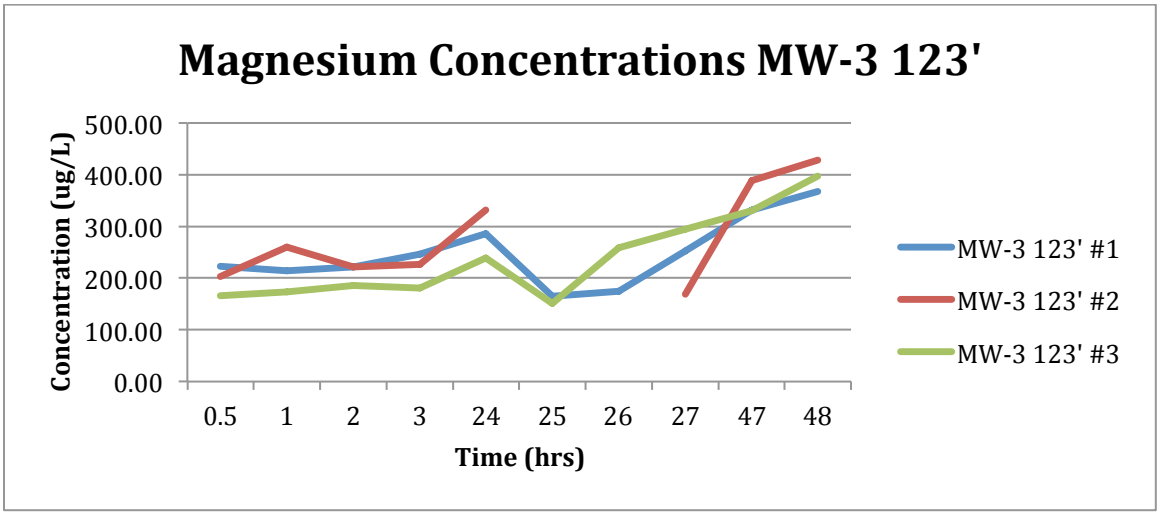
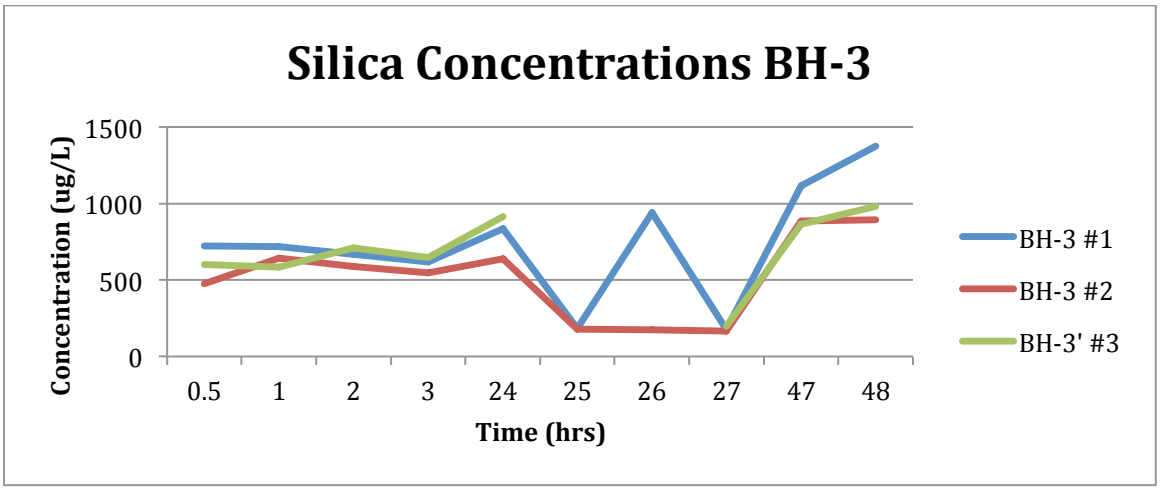
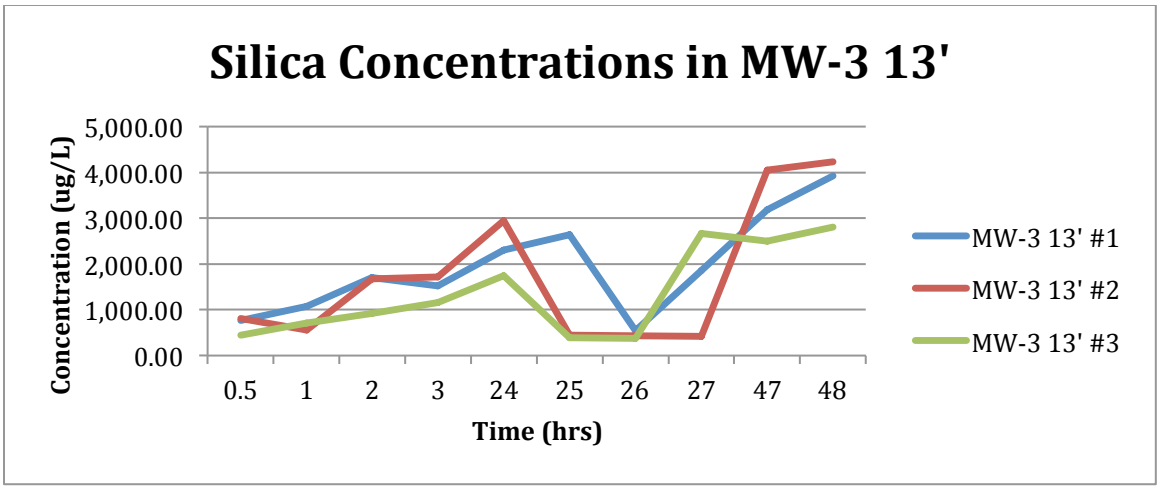


Figure 11: Magnesium concentrations from water extraction, concentrations shown in ug/L.





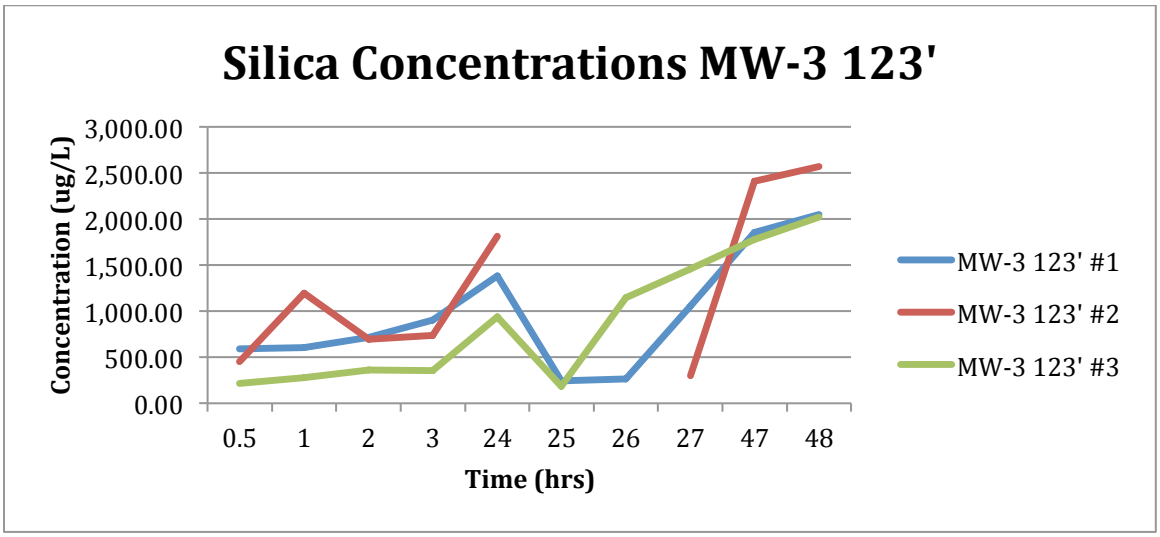
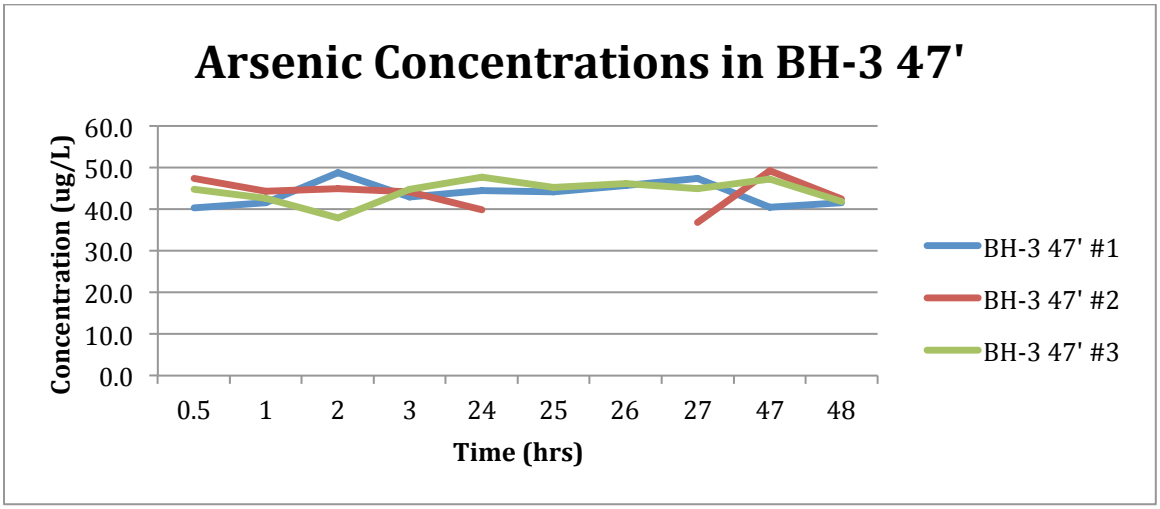


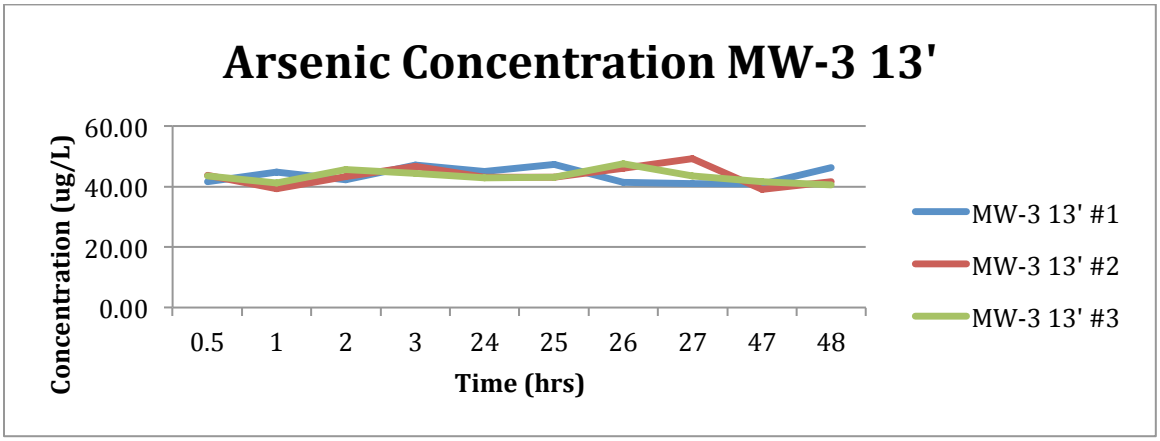
Figure 12: Concentration of Silica from the water extraction. All concentrations are shown in µg/L.

The remaining three constituents (arsenic, beryllium, and lead) exceeding the USEPA Drinking water Standards remained at fairly consistent concentrations throughout entirety of the sampling event. This suggests that there was very little happening with the analytes going into and out of solution during the sampling event. The three analytes will be discussed in more detail in the following paragraphs.

Arsenic, which has a USEPA Drinking Water Standard of 10 µg/L (USEPA Contaminants, 2015), ranged in concentration between 37.9 µg/L in BH-3 47' #2 at 2 hours and 49.2 µg/L in MW-3 123' #3 at 3 hours. There was a small amount of variability observed in all of the samples analyzed, however, nothing that appeared to be

significant based on statistical analysis. The arsenic in the study area is relatively stable, with very little arsenic going into and out of solution during the entirety of this sampling event. This is probably because the pH remained stable throughout the entirety of the sampling event. The arsenic is hypothesized to have come from nearby erosional actions (USEPA, 2015). It is unlikely that the arsenic in the project area is anthropogenic in origin. See Figure 13 for arsenic concentrations from the water extraction.





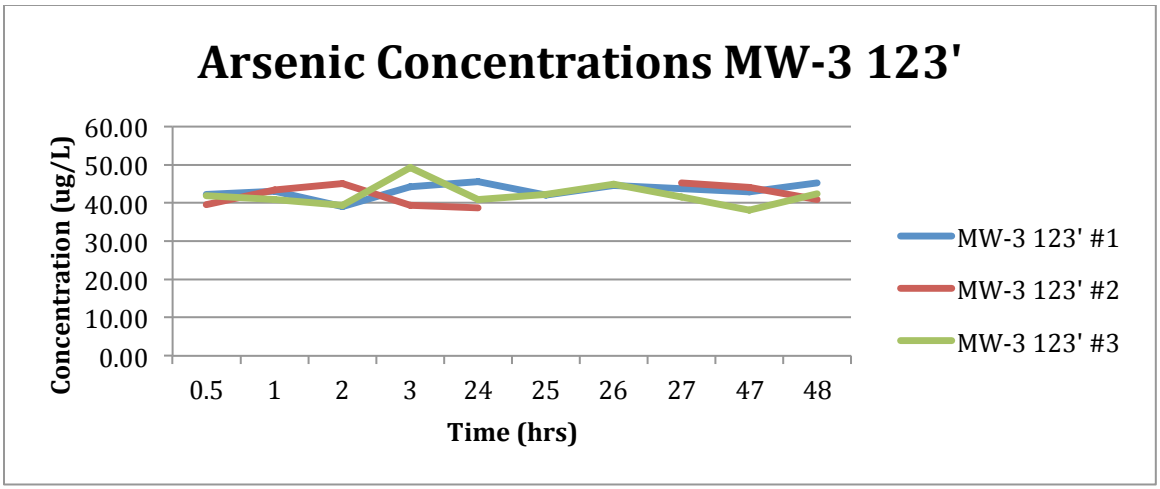
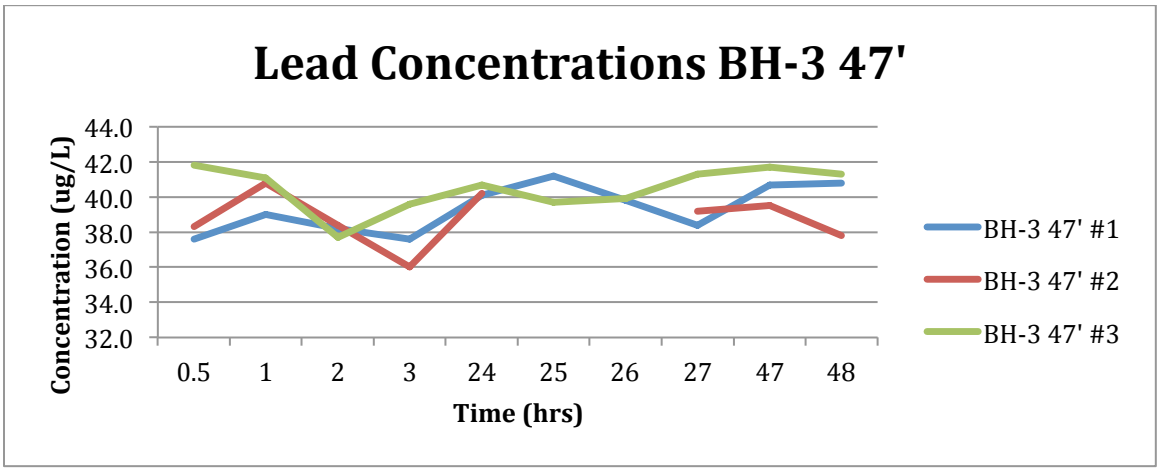
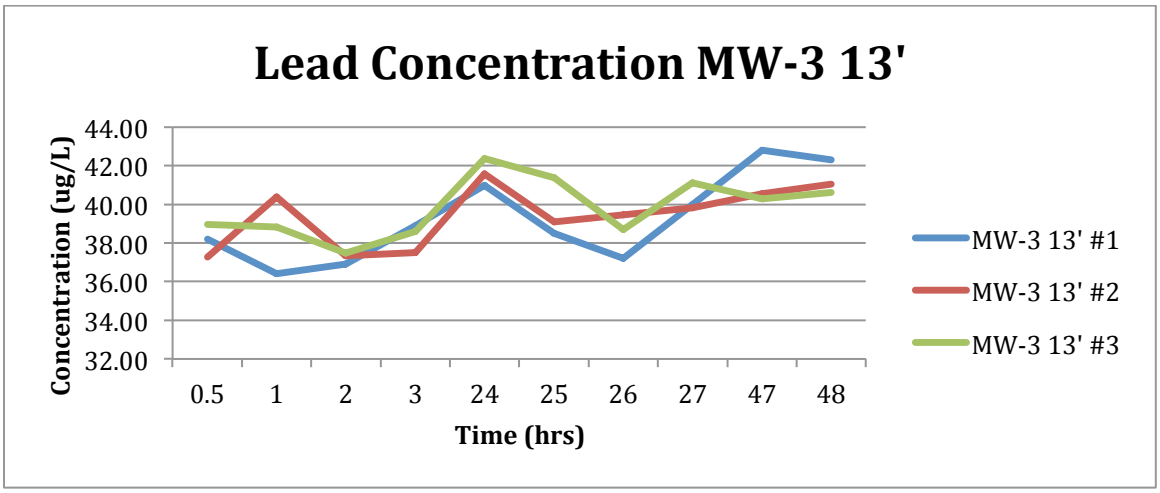


Figure 13: Arsenic concentrations from the water extraction.

Beryllium, which has a USEPA Drinking Water Standard of 4 µg/L (USEPA, 2015), ranged in concentrations between 82.2 µg/L in MW-3 13' #3 at 24 hours and 84.6 µg/L in MW-3 123' #1 at 48 hours. It is hypothesized that the beryllium concentrations were "noise" created by the ICP-OES instrument. This is thought because the only time that beryllium was detected was during the water extraction. As a confirmation the ICP-MS was used to analyze the shallow zone aquifer samples, where beryllium was found at non-detect levels.

Lead, which has a USEPA Drinking Water Standard of 15 µg/L (USEPA, 2015), ranged in concentration between 36.4 µg/L in MW-3 13' #1 at 1 hour and 42.8 µg/L in MW-3 13' #1 at 47 hours. Lead tends to be more mobile at low pH's. This means that the pH in these samples was probably more acidic. ICP-MS was used to confirm the lead results from the DI extraction (Section 7.2.2). Much like both the arsenic and beryllium there is very little variation in the lead concentrations throughout the sampling event, and the variability that is observed does not appear to be significant. It is hypothesized that the lead is from the decomposition of radionuclides associated with granitic rocks that have eroded from the nearby Sangre de Cristo Mountains (McVey, 2015). According to PHREEQ-C models the primary lead minerals in this area is cerrusite ($PbCO_3$) and anglesite ($PbSO_4$). Neither of these minerals was saturated according to the PHREEQ-C model run. It is unlikely that the lead in the project area is anthropogenic in origin.





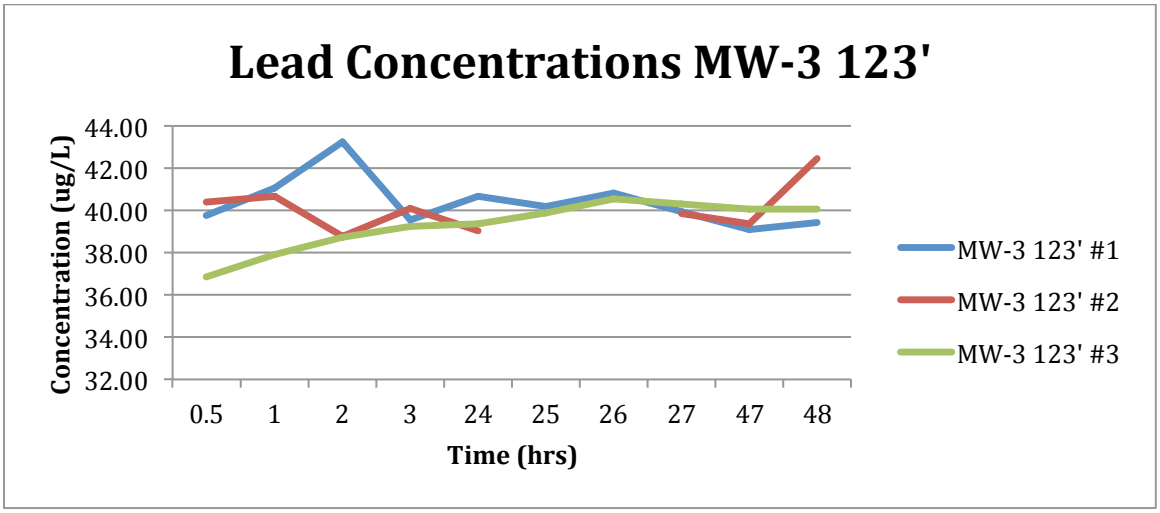


Figure 14: Lead concentrations from the water extraction.

The concentrations of the analytes that do exceed the USEPA Drinking Water Standards are at low enough concentrations, and should be easy to remove using modern water treatment techniques in order to ensure the highest quality of drinking water for the customers. See the Discussion Section for possible health effects of the analytes that exceed the USEPA Drinking Water Standards, and treatment solutions to ensure that those effects are not going to become an issue.

8.0 ICP-MS Results

In order to ensure the presence of arsenic, beryllium, lead, and uranium in the shallow zone aquifer samples were analyzed using the ICP-MS. The possibility existed that the ICP-OES method didn't have a low enough detection limit to accurately detect the compounds listed above at low concentrations. The water samples collected from MW-3, MW-4, and the Windmill Well were analyzed using the ICP-MS for the above listed metals. The ICP-MS was chosen since it has a lower detection limit for most metals, which would determine whether or not the shallow zone aquifer had detections of the selected metals at levels exceeding the USEP Drinking Water Standards.

Well	Arsenic	Beryllium	Lead	Uranium
MW-3	**14.1**	<1.0	**27.4**	28.3
MW-4	**14.6**	<1.0	**26.3**	12.1
Windmill Well	**12.8**	<1.0	**26.9**	19.3
USEPA Drinking Water Standard	10	4	15	30

Table 11: Results from of the ICP-MS, all values shown in µg/L. **Bold** values exceed USEPA Drinking Water Standards.

As shown in Table 9, only arsenic and lead where detected at levels exceeding the USEPA Drinking Water Standards. Beryllium was found to be at levels below the detection limit, and uranium was detected at levels below the USEPA Drinking Water Standard (30 µg/L) in all of the samples analyzed. This mostly confirms the water extractions; with the exception was beryllium, which was found at levels below the detection limit. Non-detect levels for beryllium with the ICP-MS confirmed the results of the ICP-OES and acid extraction results. This shows that beryllium detected during the water extraction was probably "noise" created by the instrument. The ICP-MS analysis

confirmed that both arsenic and lead are at concentrations that exceed the USEPA Drinking Water Standards in the shallow zone aquifer.

9.0 Modeling Results

The modeling that was performed was done using PHREEQ-C, which was developed by the USGS, while the Piper and Stiff Diagrams (Figures 3 and 4) were created using the Geochemist Workbench and then edited using Microsoft Powerpoint. The purpose of these models was to determine the speciation of the potentially hazardous metals that could be found in the various waters. However, it should be noted that the only metals regulated by the NMED is chromium. Hexavalent chromium (Cr VI) is highly regulated when compared to chromium-III, since Cr-VI has been shown to be acutely toxic. Additionally, knowing the valence state of the metal can give one some idea about both the solubility and mobility of the metal.

The water sample results that were modeled using PHREEQ-C included the MW-3, MW-4, and the Windmill Well, which are screened in the shallow zone aquifer. Additionally, the both of the deep zone aquifer wells, Industrial Park Well #1 and the Pow-Wow Well, were modeled using PHREEQ-C. Additionally, a mixture of waters was modeled using the PHREEQ-C modeling program. This mixture included the water from MW-4 and the 48-hour analysis from the water extraction, which is believed to be similar enough to the SJCPW to be used in the modeling, since it would take at least 48 hours or more for the SJCPW to travel through the vadose zone to the shallow zone aquifer. Unfortunately the analysis from the water extractions were analyzed using ion chromatography, due to a lack of sample volume, so the anion concentrations were interpolated and balanced using "best" judgment. Anion concentrations were hypothesized to be similar to those in the shallow zone aquifer, and then the charges were balanced to be less than 5%. These waters were modeled using mixtures consisting of 50/50, 75/25, 90/10, and 95/5 of aquifer water and extraction water mixtures respectively. The actual mixture of water in the aquifer will depend on a variety of circumstances; including what technology is used to insert the SJCPW into the aquifer, how much water is used for aquifer storage, and others factors as well. With this said the most likely

mixture to occur is the 95/5 mixture. See Appendix 4 for copies of the PHREEQ-C model outputs.

The results from the modeling of the wells were what would have been expected for fairly "fresh" waters with low concentrations of hazardous metals. The models showed that all of the concentrations of metals and any potential hazardous products that may be created were below concentrations that could be hazardous to human health. The hope was that with mixing the two different waters that the concentrations of harmful metals would be reduced to concentrations that would be below the USEPA Drinking Water Standards. It should be noted that during the run of the mixing model PHREEQ-C was unable to analyze the following elements: arsenic, beryllium, nickel, and selenium. The Wateq4f.dat database was used to perform the model runs. However, both arsenic and beryllium were found to exceed safe drinking water standards during the water extraction. With the initial water (MW-4) having a non-detect arsenic and beryllium concentration, it can be assumed that both the arsenic and beryllium concentrations will approach the safe drinking water standards. However, it is unknown at exactly what mixing ratio this will occur. Additionally, the only analytes that were analyzed during this process were the analytes that exceeded the USEPA Drinking Water Standards.

Results from the 50/50 mixture showed what was hypothesized to occur with these models. All of the concentrations of analytes diluted. Iron concentrations dropped to below the secondary USEPA Drinking Water Standards, where the modeled concentration was 200 µg/L. However, aluminum (410 µg/L) and lead (33µg/L) both remained above USEPA Drinking Water Standards, which are 50 µg/L and 15 µg/L respectively. Both arsenic and beryllium are hypothesized to have dropped since neither of these metals was detected in the aquifer waters.

Results from the 75/25 mixture once again showed all of the concentrations of analytes decreasing. Iron concentrations remained below the secondary USEPA Drinking Water Standards, where the modeled concentration was now 100 µg/L. Both aluminum (230 µg/L) and lead (27µg/L) concentrations went down, however, both

remained above the USEPA drinking water standards. Lead concentrations during this model run went down to approximately the concentration of the aquifer waters (27 μg/L), meaning that it is unlikely that the lead concentrations in the project area will go below USEPA Drinking Water Standards by dilution. It should be noted that the concentrations of both aluminum and lead went down when compared to their concentrations from the previous model run. Both arsenic and beryllium are hypothesized to have continued dropping since neither of these metals was detected in the aquifer waters.

It is hypothesized that either of the next two model runs would probably be the most realistic, with the SJCPW water making up the minority of the mixing waters. Results from the 90/10 mixture showed that once again all of the concentrations of analytes decreased. Iron concentrations remained below the secondary USEPA Drinking Water Standards, where the modeled concentration from this model was 40 μg/L. Both aluminum (120 μg/L) and lead (26μg/L) both remained above USEPA drinking water standards. Lead concentrations during this model run reached the concentrations of lead found in the aquifer waters. It should be noted that the concentrations of both of these metals went down when compared to the concentrations from the previous model run. Arsenic and beryllium are hypothesized to have continued dropped since neither of these metals was detected in the aquifer waters.

Results from the 95/5 mixture showed a continuation in the concentrations of analytes decreasing. Iron concentrations remained below the secondary USEPA Drinking Water Standards, where the modeled concentration was 20 μg/L. The aluminum (86 μg/L) and lead (26 μg/L) both remained above USEPA drinking water standards. It should be noted that the concentrations of only of aluminum went down when compared to the concentrations from the previous model run, since lead concentrations achieved aquifer levels during the previous model run. Although concentrations of aluminum didn't achieve concentrations below USEPA secondary drinking water standards during this model run, if given enough dilution aluminum concentrations would probably obtain levels below the USEPA Secondary Drinking Water Standards. Both arsenic and beryllium are hypothesized to have continued

dropping since neither of these metals was detected in the aquifer waters, it is possible that by this point that both of these metals have descended to concentrations that are below the USEPA Drinking Water Standards.

10.0 Discussion

As was expected there were several analytes that exceeded either USEPA Primary Drinking Water Standards, or USEPA Secondary Drinking Water Standards. Each of these analytes potentially can affect human in health in different ways (see above section for examples). Luckily, these analytes can easily be removed from drinking water with conventional treatment methods. These and other issues will be discussed in this section, in addition to several other issues that could be encountered by this project. These include the lack of production from the aquifer due to low hydraulic conductivities and insufficient recharge due to the lack of hydraulic conductivity.

The first issue that will be discussed will be the analytes that exceed the USEPA Secondary Drinking Water Standards. USEPA Secondary Drinking Water Standards do not tend to negatively affect human health, but instead tend to affect the aesthetic qualities of the drinking water. These qualities tend to include the color, odor, and/or taste of the drinking water. The USEPA doesn't regulate these analytes, but recommends that water providers follow these recommendations (USEPA, 2015).

There were two analytes that exceeded the USEPA Secondary Drinking Water Standards at the Project Area. These analytes were aluminum (from the water extraction and the shallow zone aquifer) and iron (from the water extraction).

According to the USEPA aluminum tends to affect the color of drinking water more than anything (USEPA, 2015). However, if consumed in high enough concentrations aluminum can cause nausea, vomiting, mouth ulcers, skin ulcers, and arthritic pain (Chanban et al, 1998). There are rumored links between excessive consumption of aluminum and Alzheimer's, however according to the World Health Organization these two attributes have been inconclusively linked (Chanban et al, 1998).

Luckily conventional treatment methods such as filtration, coagulation, aeration, and/or activated carbon are able to remove most of the aluminum from the drinking water. Water filtration involves having the water pass through filters made of sand, gravel, or charcoal, which helps to remove small particles (EPA, 2015). Coagulation removes dirt and other particles suspended in water. Alum and other chemicals are added to water to form tiny sticky particles called "floc" which attract the dirt particles. The combined weight of the dirt and the alum (floc) become heavy enough to sink to the bottom during sedimentation (EPA, 2015). Aeration involves either pumping air or cascading the water out of a facet, which is effective at removing any contaminates that have the potential of volatilizing (EPA, 2015).

Iron is considered to be hazardous to human health if taken in high enough doses. However, complications rarely, if ever, arise from iron in drinking water since only about 5% of iron consumed by Americans is supplied by tap water (IDPH, 2015). Iron may not negatively affect human health, and is necessary for good health and oxygen transportation in blood (IDPH, 2015). However, iron can have a drastic affect on the aesthetic qualities of drinking water. These aesthetic effects can include a reddish color and a disagreeable metallic taste, as well as turning beverages and vegetables a dark color and staining fixtures. Luckily, like aluminum, iron is easily removed using conventional treatment methods such as using a manganese greensand filter, catalytic filtration, and/or aeration/filtration are able to remove most of the iron from the drinking water. Manganese greensand is a natural and/or artificial mineral that when treated with potassium permanganate is capable of removing iron from drinking water. This process is effective at removing dissolved iron from drinking water, however it does require chemical regeneration (IDPH, 2015). Catalytic filtration, involves a granular filter medium that enhances the reaction between oxygen and iron and then filters the insoluble iron (IDPH, 2015).

USEPA Primary Drinking Water Standards were established to protect human health. The USEPA does regulate these analytes, and all of the regulations for each

analyte should be followed in order to protect human health and ensure that the water providers don't face heavy fines.

Five analytes exceeded the USEPA Primary Drinking Water Standards in the Project Area. These analytes were arsenic (water extraction and deep zone aquifer), beryllium (water extraction), fluoride (deep zone aquifer), lead (water extraction and shallow zone aquifer), and nitrates (shallow zone aquifer). The following paragraphs will discuss the possible health effects of these analytes and how to remove them from drinking water.

According to the USEPA long-term health effects from drinking elevated levels of arsenic in drinking water include skin damage, circulatory problems, and/or an elevated risk of getting cancer (USEPA Arsenic, 2015). These ailments tend to take years of drinking water with elevated arsenic levels to appear. Luckily arsenic can be easily removed to be below the maximum contaminant level (MCL) with standard water treatment methods: which includes ion exchange, filtration, and/or reverse osmosis. Ion exchange (IX) is a physical-chemical process in which ions are swapped between a solution phase and solid resin phase. If As(III) is present, it must be oxidized to As(V) in order for IX to be effective. The solid resin is typically an elastic three-dimensional hydrocarbon network containing a large number of ionizable groups electrostatically bound to the resin. These groups are exchanged for ions of similar charge in solution that have a stronger exchange affinity (i.e., selectivity) for the resin (USEPA, 2015). Reverse osmosis units force water through a semi-permeable membrane under pressure, leaving contaminants behind. A down side to reverse osmosis units is that they use approximately three times as much water as other more efficient methods to treat (USEPA, 2015).

According to the USEPA long-term health effects from drinking water with elevated levels of beryllium include the possible development of intestinal lesions. Like arsenic the health effects of beryllium take years to appear. Additionally, like arsenic, beryllium can be removed from water be to below the MCL with using standard treatment techniques including ion exchange, filtration, and/or reverse osmosis. Using

one or more of these techniques should be able to remove enough beryllium to make the drinking water safe for human consumption. One thing that should be noted about the beryllium concentrations from the water extraction is that there is the possibility that it could be "noise". This is stated because the ICP-OES isn't the best at detecting beryllium. Additionally, the lowest beryllium standard was 1ppm while the highest beryllium detection was 0.08ppm, well below the standard. For this reason the shallow zone groundwater samples were analyzed for beryllium on the ICP-MS. This round of analysis showed beryllium at levels below the detection limit of the ICP-MS. This says that there is the possibility that beryllium concentrations are at lower levels than what are reported in the sections above.

According to the USEPA elevated levels of fluoride effect children, specifically 8 and younger, and adults differently. In children the effects of elevated levels of fluoride include developing pits in the enamel of their teeth, and several other cosmetic effects on teeth. In adults elevated levels of fluoride could increase the likelihood of getting a bone fracture, and could also lead to effects on bones leading to pain and tenderness. However, a little fluoride (approximately 2 mg/L or less) in the drinking water is a good thing since it helps to strengthen the enamel on teeth. Luckily, fluoride concentrations are easily lowered to the MCL by using standard treatment techniques including distillation and/or reverse osmosis. Distillation is the process in which water is heated and run through glass tubing where it is allowed to re-condense, this re-condensed water tends to be lower in contaminates since most contaminates are unable to evaporate with the water (USEPA, 2015). Using one or more of these methods should lower the fluoride level enough to make the drinking water safe for human consumption.

According to the USEPA, much like fluoride, there are differing health effects for infants, children, and adults. In infants, the health effects from drinking water with elevated lead concentrations could include a delay in physical and/or mental development. In children, the possible health effects include deficits in attention span and learning abilities. While in adults, the potential health effects could include kidney problems and/or high blood pressure. With the exception of infants and children, the

health effects could take years to develop. Lead is an interesting issue when it comes to drinking water, since the primary source of lead in drinking water tends to come from lead pipes. Therefore the USEPA recommends flushing the system for 30 seconds to "flush" the lead from the drinking water. However, if that isn't the source of the lead should be able to be filtered from the drinking water using a carbon filters or ion exchange resins in order to bring the lead concentration down below the MCL.

According to the USEPA nitrate is a contaminant that primarily effects infants below six months in age. If infants drinking water containing nitrates above the MCL for an extended period of time, they have the potential of developing "blue baby" syndrome, which could lead to the death of the infant by suffocation. Luckily, there are standard treatments that remove nitrates to below the MCL, which include reverse osmosis, ion exchange, and/or electrodialysis. Electrodialysis is used to transport salt ions from one solution through ion-exchange membranes to another solution under the influence of an applied electric potential difference (USEPA, 2015). Any of these methods should be able to remove enough nitrates to make the drinking water safe for human consumption.

As read above, removing various contaminates with modern techniques is relatively easy and mostly inexpensive. For this project a combination of ion exchange and filtration would remove most of the contaminates associated with this project. However, upon concentration of some of the above mentioned contaminants would concentrate them to the point of being a hazardous material, this would raise the cost of treating the water.

However, there are additional issues that it must overcome in order for the water production of the aquifer to be viable. Although it is not the primary focus of this paper, a small section will be dedicated to these obstacles. According to hydraulic conductivity numbers determined by DBS&A and tritium numbers calculated by the USGS National Water Quality Laboratory, the groundwater beneath the Project Area is moving slow. This also tends to suggest that the recharge values, if the water were to recharge via surface infiltration, when water is put on the surface and allowed to seep into the ground,

would be slow as well. Luckily there are technological advances that have been made to overcome these obstacles.

The first issue that will be dealt with is the slow infiltration rate. Increasing the infiltration of this project can be overcome in numerous different ways, however, only three will be discussed. The three methods that will be discussed are infiltration galleries, injection wells, and the construction of headwalls. Infiltration galleries are horizontal pipes that are usually placed approximately 2 meters below the ground surface. This would lead to a reduction in evaporation, but for this project probably wouldn't lead to the increased head that would be required for the SJCPW to make it all of the water to the aquifer. The next solution could potentially come from the installation of injection wells. These would allow the injection of the SJCPW directly into the aquifer. This would be efficient since it would allow the water to be injected directly into the aquifer. The final solution this paper will offer for this issue is the construction of a headwall. A headwall is a concrete wall that allows for the redirection of water flow. In this case a headwall would allow the SJCPW to obtain the proper head in order for the SJCPW to make it to the aquifer, however, there would probably still be some water losses to evapotranspiration. Any of these solutions would solve the lack of recharge issue faced by this project. However, some of these solutions would work better than others. In this case the infiltration gallery would probably work best, by being able to use a larger area to direct the SJCPW downward to the shallow zone aquifer.

The next issue faced by this project is the lack of permeability within the aquifer itself. This issue is easily solved in a couple of different ways. The first way would be to have a very large screened interval in the production well(s). This interval could be hundreds of feet into the thousands of feet to ensure that the well would be able to supple adequate water for the public. However, the screen length for the production wells would depend on how deep the aquifer is in this zone. The next thing that would have to be done is installing a large enough pump to ensure adequate product from the well. These solutions would help the aquifer to produce enough volume to provide drinking water to the intended customers.

11.0 Conclusions

As of the writing of this paper the issues that have been addressed by this paper can easily be taken care of. Increased screen lengths in the production wells to ensure that there is enough production from the wells, enhanced water treatment in order to ensure good water quality for the recipients of the water, to creating an infiltration gallery and/or drilling injection wells to ensure that the SJCPW makes it to the aquifer. With all of these "issues" cleared up from a water quality and production standpoint it would seem like this project should easily be scheduled to move forward.

At this time the Bureau of Reclamation is unsure if they are going to move forward with this project. They would prefer to treat the SJCPW only once as they extract it from the river, and then not to have to treat the water again when they extract it from the ground as drinking water. According to the results of this study it appears that the double treatment option is want they will be required to do to meet USEPA Drinking Water Standards. However, if they decide to move forward with this project, poor water quality should not be an issue that will be hard time to deal with. Modern water treatment methods will be able to bring the mixed aquifer and SJCPW water up to the USEPA Drinking Water Standards, ensuring the safety of this water for human consumption.

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BH-3

N: 35 51' 57.26"
W: 106 2' 36.05"

GEOLOGIC BORING/WELL LOG

Project #:	Project Name: Pojoaque ASR	Boring/Well #: BH-3
Geologist: R. Carruth	Driller/Company: USGS Research Drilling	
Drilling Equip.: Auger Rig	Date Start: 11/17/14	Date Completed: 11/19/14
Surface Elev.: 5979.33 ft	Top of Casing Elev.: n/a	Total Depth (ft): 61.5 BLS / Well Depth: N/A

Method of Drilling
- ☒ Hollow Stem w/ corebarrel ☐ Direct Rotary
- ☐ Air Rotary ☐ Bucket Auger
- ☐ MUD Rotary ☐ Flight Auger
- Hole Diameter: 8 5/8-inch 3-inch core

Casing/Riser Type N/A
- ☐ Steel ☐ Threaded
- ☐ Galv ☐ Welded
- ☐ PVC ☐ Solvent
- ☐ SS ☐ Welded
- Drive Shoe? ☐ Yes ☐ No
- Height above/below surface: ____
- Diameter: ____

Screen Portion of Well N/A
- Material ____
- Diameter ____ Length ____
- Set between ____ ft and ____ ft
- Slot size ____

Filter Pack N/A
- Size ____
- Method of Install ____
- Composition ____
- Volume Used ____
- Depth to top of f.p. ____

Annulus Seal N/A
- ☐ Bentonite Pellets ____ Chips ____
- ☐ ____
- Volume Used? ____
- Method of Instal. ____
- Depth: from ____ ft. to ____ ft.

Grout seal/fill open hole
- Used? ☒ Yes ☐ No Volume ____
- ☐ Neat Cement ☒ Bentonite
- ☐ Geothermal grout
- Method of Instal. Displacement w/ auger removal
- Depth: from 1 ft. to 61.5 ft.

Well Head Completion N/A
- ☐ Flushmount ☐ Stand Up
- Cap Type ____
- Lock # ____
- Volume Used ____

Development N/A
- Method ____
- Gallons Evacuated ____
- Date ____
- Odor ____

Static Water Level
- Initial 49.25 ft bls
- Development ____ ft.
- 24 hr. 49.1 ft. bls (16)

DRILLING		SAMPLE							GEOLOGIC LOG		Bore Hole Description
Depth (ft)	PID Reading (ppm)	Sample Type	Sample ID	Blow Count 0-6"	6-12"	12-18"	18-24"	Recovery-(in)	USCS Class	Contact-Depth	Descriptions and Comments
0											Augered to 61.5 ft. bls, obtained continuous 3-inch core, recorded dtw after 15+ hours, removed auger flights and sealed bore hole with geothermal grout.
											Tan to light brown, unconsolidated to loosely consolidated, medium to very coarse arroyo sands with gravel and larger cobbles. Larger grains are sub-angular to angular. Zones of weak cementation effervesce moderately with 5% HCl
			10-11 ft Geochemistry sample zone #1								
20											

GEOLOGIC BORING/WELL LOG

Project #:	Project Name: Pojoaque ASR	Boring/Well #: BH-3	
Geologist: R. Carruth	Driller/Company: USGS Research Drilling		
Drilling Equip.: Auger Rig		Date Start: 11/17/14	Date Completed: 11/19/14
Surface Elev.:	Top of Casing Elev.:	Total Depth (ft): 61.5	Well Depth: N/A

DRILLING		SAMPLE							GEOLOGIC LOG		
				Blow Count							
Depth (ft)	PID Reading (ppm)	Sample Type	Sample ID	0-6"	6-12"	12-18"	18-24"	Recovery-(in)	USCS Class	Contact-Depth	Descriptions and Comments
20											Continued arroyo sands and gravels with increasing zones of cementation and presence of $CaCO_3$ deposition. Cemented core effervesces moderately to strongly with 5% HCl.
			21 ft Geochemistry Sample Zone #2								
23.5	←		Geochem. Sample Zone #3 Contact w/ Tusuque Fm. and/or sediments weathered from Tusuque								At 23.5 ft bls, contact with fine-grained Tusuque Formation (?) Core is light brown to brown, loosely to moderately consolidated, fine sands and silt w/ areas of some clay content. Core material weakly to moderately effervesces with 5% HCl. Core also has some water content but not saturated.
46											Zone of decreased fines and increased coarse sands and gravel. First zone of saturation. Paused drilling to measure dtw. dtw = 47.6 ft bls after 35 min.
			47-48 Geochem. Sample Zone #4								
			47.5 – First measurable dtw								
48.5											

GEOLOGIC BORING/WELL LOG

Project #:	Project Name: Pojoaque ASR	Boring/Well #: BH-3	
Geologist: R. Carruth	Driller/Company: USGS Research Drilling		
Drilling Equip.: Auger Rig		Date Start: 11/17/14	Date Completed: 11/19/14
Surface Elev.:	Top of Casing Elev.:	Total Depth: 61.5 (ft)	Well Depth: N/A

DRILLING		SAMPLE								GEOLOGIC LOG		
				Blow Count								
Depth (ft)	PID Reading (ppm)	Sample Type	Sample ID	0-6"	6-12"	12-18"	18-24"	Recovery-(in)	USCS Class	Contact-Depth	Descriptions and Comments
48.5											Fully saturated, light brown to brown, weakly to moderately consolidated, fine sands and silt with zones of increasing clay content. Core also has zones of strongly consolidated fine sand and siltstone. Material generally does not effervesce with 5% HCL. DTW after 16 hours = 49.10 ft bls.
	49.10 – dtw below approx surface after 16 hours.										
	60.5-61.5 Geochem. Sample Zone #5										
61.5											

BH-4

N: 35 51' 44.16"
W: 106 2' 34.52"

GEOLOGIC BORING/WELL LOG

Project #:	Project Name: Pojoaque ASR	Boring/Well #: BH-4
Geologist: R. Carruth	Driller/Company: USGS Research Drilling	
Drilling Equip.: Auger Rig	Date Start: 11/11/14	Date Completed: 11/13/14
Surface Elev.: 6048.88 ft	Top of Casing Elev.: n/a	Total Depth: 69.5 ft / Well Depth:

Method of Drilling
- [x] Hollow Stem w/ core barrel
- [ ] Direct Rotary
- [ ] Air Rotary
- [ ] Bucket Auger
- [ ] MUD Rotary
- [ ] Flight Auger

Hole Diameter: 8 5/8 in. 4 1/4 in. ID, 3 in. core

Casing/Riser Type N/A
- [ ] Steel [ ] Threaded
- [ ] Galv [ ] Welded
- [ ] PVC [ ] Solvent
- [ ] SS [ ] Welded

Height above/below surface: ____
Diameter: ____
Drive Shoe? [ ] Yes [ ] No

Screen Portion of Well N/A
Material: ____
Diameter ____ Length ____
Set between ____ ft and ____ ft
Slot size ____

Filter Pack N/A
Size ____
Method of Install ____
Composition ____
Volume Used ____
Depth to top of f.p. ____

Annulus Seal N/A
- [ ] Bentonite Pellets ____ Chips ____
- [ ] ____

Volume Used? ____
Method of Instal. ____
Depth: from ____ ft. to ____ ft.

Grout - seal open hole
Used? [x] Yes [ ] No Volume ____
- [ ] Neat Cement
- [x] Bentonite
- [x] Geothermal grout

Method of Instal. displacement w/ auger removal
Depth: from 1 ft. to 69.5 ft.

Well Head Completion N/A
- [ ] Flushmount
- [ ] Stand Up

Cap Type ____
Lock # ____
Volume Used ____

Development N/A
Method ____
Gallons Evacuated ____
Date ____
Odor ____

Static Water Level
Initial n/a due to low permeability sandy clay ft
Development ____ ft.
24 hr. 58.03 ft. bls
1.5

DRILLING / SAMPLE / GEOLOGIC LOG — Bore Hole Description

Depth (ft)	PID Reading (ppm)	Sample Type	Sample ID	Blow Count 0-6"	6-12"	12-18"	18-24"	Recovery-(in)	USCS Class	Contact-Depth	Descriptions and Comments
											Augered to 69.5 ft bls, obtained continuous 3-in. core, obtained dtw after 15 hours, removed auger flights and sealed hole with thermally conductive grout (geothermal grout)
0											Light tan to reddish brown medium to very coarse sand with gravel. Grains are rounded to angular.
2.5											
2.5											Light tan to reddish brown medium to very coarse sand with gravel. Sub angular to angular grains with zones of strong cementation that effervesces moderately w/ 5% HCl.
5.5											

Specific Conductance of sample from 2.5 ft — unfiltered 1:1 ratio w/ DI water = 86.1 µs/cm

GEOLOGIC BORING/WELL LOG

Project #:	Project Name: Pojoaque ASR	Boring/Well #: BH-4
Geologist:	Driller/Company:	
Drilling Equip.:	Date Start:	Date Completed:
Surface Elev.:	Top of Casing Elev.:	Total Depth: / Well Depth:

DRILLING		SAMPLE							GEOLOGIC LOG		
				Blow Count							
Depth	PID Reading (ppm)	Sample Type	Sample ID	0-6"	6-12"	12-18"	18-24"	Recovery-(in)	USCS Class	Contact-Depth	Descriptions and Comments
5.5											Tan to reddish brown medium to very coarse unconsolidated sand with gravel and large cobbles of quartz and feldspar w/ mica and green crystalline inclusions.
16.5											Reddish brown to brown fine to coarse sand with cobbles of crystalline rock - quartz and darker mafic minerals
17.5											Brown to reddish brown very fine to very coarse sand. Sub angular to angular grains.
		19-20 ft Geochemistry sample-zone #1									
20.5											Light brown to brown very fine to coarse sand with minor silt. Some weak cementation that effervesces moderately w/ 5% HCL.
21.5											Tan to reddish brown fine to very coarse sand with cobbles of crystalline rock (quartz and feldspar) w/ mica inclusions. Mild effervescence of weakly cemented sediment.
26.5											

GEOLOGIC BORING/WELL LOG

Project #:	Project Name: Pojoaque	Boring/Well #: BH-4
Geologist:	Driller/Company:	
Drilling Equip.:	Date Start:	Date Completed:
Surface Elev.:	Top of Casing Elev.:	Total Depth: / Well Depth:

DRILLING		SAMPLE							GEOLOGIC LOG		
				Blow Count							
Depth	PID Reading (ppm)	Sample Type	Sample ID	0-6"	6-12"	12-18"	18-24"	Recovery-(in)	USCS Class	Contact-Depth	Descriptions and Comments
26.5											Brown to dark brown weakly consolidated fine to medium sand with minor coarse sand and gravel. Weak effervescence with 5% HCL
27.5											Brown to dark brown weakly consolidated silty fine to medium sand
29.5		28-29 ft Geochemistry Sample Zone #2									Light brown to reddish brown medium to very coarse sand. Areas of weak consolidation that moderately effervesce with 5% HCL. Some coarse sand and gravel grains show yellowish-orange staining
		30-31 ft Geochemistry Sample Zone #3									
33											weakly consolidated tan to brown fine to coarse sand with dark yellowish to orange staining. Consolidated material moderately effervesces with 5% HCL.
36											Tan to light brown unconsolidated to weakly consolidated medium to very coarse sand with gravel and large cobbles of quartz and feldspar with mica.
41											

GEOLOGIC BORING/WELL LOG

Project #:	Project Name:	Boring/Well #: BH-4
Geologist:	Driller/Company:	
Drilling Equip.:	Date Start:	Date Completed:
Surface Elev.:	Top of Casing Elev.:	Total Depth: / Well Depth:

DRILLING		SAMPLE							GEOLOGIC LOG		
				Blow Count							
Depth	PID Reading (ppm)	Sample Type	Sample ID	0-6"	6-12"	12-18"	18-24"	Recovery-(in)	USCS Class	Contact-Depth	Descriptions and Comments
41											Light Tan to brown, unconsolidated to weakly consolidated fine to coarse sand. Zones of weakly consolidated fine to medium sand do not effervesce with 5% HCL. Unconsolidated material also contains very coarse sand and small sub angular to rounded cobbles.
		50-51 Geochemistry Sample Zone #4									
51.25											At 51.25 ft below land surface, contact with weakly to moderately consolidated fine to very fine sand and silt with some clay. Zones of core stained white show moderate effervescence with 5% HCL. Core sections show increasing saturation below 51.25 ft and exhibit swelling inside core baccals. Borehole dry upon completion. After 15 hours, water level measured at 58.03 ft below land surface.
		56-57 ft Geochemistry Sample Zone #5									
		DTW = 58.03 ft/s 11/12/14 @ 0740									
69.5 bottom of bore hole											

Contact at 51.25

N: 35 52' 10.73"
W: 106 2' 42.69"

MW-3

GEOLOGIC BORING/WELL LOG

Project #:	Project Name: Pojoaque ASR	Boring/Well #: MW-3
Geologist: R. Carruth	Driller/Company: USGS Research Drilling	
Drilling Equip.: Auger Rig	Date Start: 11/20/14	Date Completed: 11/22/14
Surface Elev.: 5961.52 ft	Top of Casing Elev.: 5964.04 ft	Total Depth: 129 (ft) / Well Depth: 129 (ft)

Method of Drilling

☒ Hollow Stem w/ core barrel ☐ Direct Rotary
☐ Air Rotary ☐ Bucket Auger
☐ MUD Rotary ☐ Flight Auger
Hole Diameter: 8 5/8 inch w/ 3-inch core

Casing/Riser Type

☐ Steel ☐ Threaded
☐ Galv ☐ Welded
☒ PVC ☐ Solvent
☐ SS ☐ Welded
Drive Shoe? ☐ Yes ☐ No
Height above/below surface: 30-inch above / 129 ft below
Diameter: 2-inch

Screen Portion of Well

Material: PVC
Diameter: 2-inch Length: 20 ft
Set between: 104 ft and 124 ft
Slot size: 0.10

Filter Pack

Size: 0-10 2
Method of Install: surface pour w/ depth sounding
Composition: sand
Volume Used: 18 bags
Depth to top of f.p.: 99-129 ft

Annulus Seal

☒ Bentonite Pellets ☐ Chips
☐ 1/4-inch pellets
Volume Used? 5 5-gal. buckets
Method of Instal.: surface pour
Depth: from 99 ft. to 90.6 ft.

Grout

Used? ☒ Yes ☐ No Volume: 39 bags
☐ Neat Cement ☒ Bentonite
☐
Method of Instal.: surface pour
Depth: from 90.6 ft. to 3 ft.

Well Head Completion: 4'x4' cement pad

☐ Flushmount ☒ Stand Up
Cap Type: 8-inch locking
Lock #:
Volume Used: 8 bags cement

Development

Method: balling
Gallons Evacuated: 200
Date: 11/22 & 11/23
Odor: none

Static Water Level

Initial: 115.21 ft bls @ 1705 11/21/14
Development: ____ ft.
24 hr. 109.55 ft. bls @ 0635 11/22
13

DRILLING		SAMPLE							GEOLOGIC LOG Bore Hole Description		
Depth (ft)	PID Reading (ppm)	Sample Type	Sample ID	Blow Count 0-6"	6-12"	12-18"	18-24"	Recovery-(in)	USCS Class	Contact-Depth	Descriptions and Comments
0											Augered to 129 ft bls, obtained continuous 3-inch core from 0-124 ft. DTW after 13 hrs = 109.55 ft bls. Removed auger flights on 11/22/14 and constructed monitor well with 2-inch PVC.
											Tan to light brown, unconsolidated to loosely consolidated fine sand and silt with ~10% medium to very coarse sand. Consolidated material also contains ~2% gravel inclusions and moderately to strongly effervesces with 5% HCl.
8											

GEOLOGIC BORING/WELL LOG

Project #:	Project Name: Pojoaque ASR	Boring/Well #: MW-3
Geologist:	Driller/Company:	
Drilling Equip.:	Date Start:	Date Completed:
Surface Elev.:	Top of Casing Elev.:	Total Depth: / Well Depth:

DRILLING		SAMPLE							GEOLOGIC LOG		
Depth (ft)	PID Reading (ppm)	Sample Type	Sample ID	Blow Count 0-6"	6-12"	12-18"	18-24"	Recovery-(in)	USCS Class	Contact-Depth	Descriptions and Comments
8											Transition from largely fine-grained sediments to medium to very coarse sand with gravel and larger cobbles of granitic rock
10											Transition back to largely fine-grained sediments - unconsolidated to loosely consolidated fine sand and silt
13											Transition back to unconsolidated sands - fine to very coarse with gravel and cobbles
	13.5-14.5		Rock Chemistry Sample Zone 1								
14.5			Probable contact with Tesuque Fm.								Begin thick sequence of fine-grained sediments. Light tan to greyish tan to light brown weakly to moderately consolidated fine sand and silt with zones of minor clay. Consolidated sediments effervesce moderately with 5% HCL. Sequence appears to be largely dry
36											

GEOLOGIC BORING/WELL LOG

Project #:	Project Name: Pojoaque ASR	Boring/Well #: MW-3
Geologist:	Driller/Company:	
Drilling Equip.:	Date Start:	Date Completed:
Surface Elev.:	Top of Casing Elev.:	Total Depth: / Well Depth:

DRILLING		SAMPLE							GEOLOGIC LOG		
				Blow Count							
Depth (ft)	PID Reading (ppm)	Sample Type	Sample ID	0-6"	6-12"	12-18"	18-24"	Recovery-(in)	USCS Class	Contact-Depth	Descriptions and Comments
36											Continued sequence of fine-grained sediments. Moisture content first noticed at 36 ft and continues with a moderate darkening of the sediments with depth.
	42-43		Rock Chemistry Sample Zone 2 - zone of $CaCO_3$ deposition.								
90											Contact with a tan to light brown sandstone - hard drilling effervesces with 5% HCL
91											Continued sequence of fine-grained sediments with moisture content increasing continually, evidenced by visable wetness and darker color of sequence
	93-94		Rock Chemistry Sample Zone 3 - zone of increased moisture content - dark brown sandy silt								
115											Fully saturated loosely consolidated fine/medium sand and sandy silt - sediments are dark brown with water content.
	114.5-115.5		Rock Chemistry Sample Zone 4 - Top of water bearing zone.								
											Contact with sandstone facies at 124 - unable to advance auger with core barrel. Total depth of 129 ft reached with replacing core barrel with an inner drill bit.
124	123-124		Sample Zone 5								

N: 35 51' 57.26"
W: 106 2' 36.05"

MW-4

GEOLOGIC BORING/WELL LOG

Page 1 of 4

Project #:	Project Name: Pojoaque ASR	Boring/Well #: MW-4
Geologist: R. Carruth	Driller/Company: USGS Research Drilling	
Drilling Equip.: Auger Rig	Date Start: 11/14/14	Date Completed: 11/17/14
Surface Elev.: 6009.12 ft	Top of Casing Elev.: 6011.32 ft	Total Depth: 88.5 (ft) / Well Depth:

Method of Drilling

- ☒ Hollow Stem w/ corebarrel ☐ Direct Rotary
- ☐ Air Rotary ☐ Bucket Auger
- ☐ MUD Rotary ☐ Flight Auger

Hole Diameter: 8 5/8 - in. w/ 3-inch core

Casing/Riser Type

- ☐ Steel ☐ Threaded
- ☐ Galv ☐ Welded
- ☒ PVC ☐ Solvent
- ☐ SS ☐ Welded

Drive Shoe? ☐ Yes ☐ No

Height above/below surface: 30-inch above / 85 ft below

Diameter: 2-inch

Screen Portion of Well

Material: PVC

Diameter: 2-inch Length: 35 ft

Set between: 45 ft and 80 ft

Slot size: 0.10

Filter Pack

Size: 0.1020

Method of Install: surface pour with depth sounding

Composition: sand

Volume Used: 30.5 bags

Depth to top of f.p.: 40 - 88.5

Annulus Seal

☒ Bentonite Pellets X ☐ Chips

☐ 1/4-inch pellets

Volume Used? 4 5 gal buckets

Method of Instal.: surface pour

Depth: from 40 ft. to 33.2 ft.

Grout

Used? ☒ Yes ☐ No Volume: 14 bags

☐ Neat Cement ☒ Bentonite

☐

Method of Instal.: surface pour

Depth: from 33.2 ft. to 2.5 ft.

Well Head Completion 4x4' cement pad

☐ Flushmount ☒ Stand Up 30-inch

Cap Type: 8-inch locking

Lock #:

Volume Used: 8 bags cement

Development

Method: bailing

Gallons Evacuated: 200

Date: 11/16 & 11/17

Odor: none

Static Water Level

Initial: 61.45 ft 11/15 @ 1424

Development: ____ ft.

24 hr.: 53.72 ft. bls 11/16 @ 0915

45

DRILLING		SAMPLE							GEOLOGIC LOG		Bore Hole Description
Depth (ft)	PID Reading (ppm)	Sample Type	Sample ID	Blow Count 0-6"	6-12"	12-18"	18-24"	Recovery-(in)	USCS Class	Contact-Depth	Descriptions and Comments
0		MW-4		located on terrace above arroyo							Tan to light brown loosely consolidated fine sand to silt with ~10% medium to very coarse sand. Consolidated material effervesces moderately to strongly with 5% HCL Minor (~2%) gravel also present in consolidated material.
9.5											

Augered to 88.5 ft bls, obtained continuous 3-inch core. Obtained dtw 15 hrs after reaching total depth. Removed auger flights and constructed well w/ 2" PVC.

MW-4

GEOLOGIC BORING/WELL LOG

Project #:	Project Name: Pojoaque ASR	Boring/Well #: MW-4
Geologist:	Driller/Company:	
Drilling Equip.:	Date Start:	Date Completed:
Surface Elev.:	Top of Casing Elev.:	Total Depth: / Well Depth:

DRILLING		SAMPLE							GEOLOGIC LOG		
				Blow Count							
Depth	PID Reading (ppm)	Sample Type	Sample ID	0-6"	6-12"	12-18"	18-24"	Recovery-(in)	USCS Class	Contact-Depth	Descriptions and Comments
9.5			Arroyo Sands								Tan to light brown, fine to very coarse sand with gravel. Material is unconsolidated and appears to be the same as the arroyo surface material. Coarse sand and gravel is sub-rounded to angular and appears to be composed primarily of quartz, feldspar, and some darker mafic minerals.
			12-13 ft Geochemistry Sample Zone #1								
13.5											Tan to light brown loosely to moderately consolidated fine sand/silt with about 5-10% coarser sand and gravel. Material weakly to moderately effervesces with 5% HCL
22											Zone of strongly cemented coarse-grained sands and gravels that strongly effervesce with 5% HCL
23											

GEOLOGIC BORING/WELL LOG

Project #:	Project Name: Pojoaque ASR	Boring/Well #: MW-4
Geologist:	Driller/Company:	
Drilling Equip.:	Date Start:	Date Completed:
Surface Elev.:	Top of Casing Elev.:	Total Depth: / Well Depth:

DRILLING		SAMPLE							GEOLOGIC LOG		
				Blow Count							
Depth	PID Reading (ppm)	Sample Type	Sample ID	0-6"	6-12"	12-18"	18-24"	Recovery-(in)	USCS Class	Contact-Depth	Descriptions and Comments
23											Tan to light brown, largely unconsolidated medium sand to silt. Material strongly effervesces with 5% HCL.
27											Tan to light brown to reddish brown loosely to strongly consolidated fine sand and silt. Lighter material weakly effervesces with 5% HCL Moisture content first noticed at 36.5 ft and increases with depth to 63.5 ft
			36-37 ft Geochemistry Sample Zone #2								
			53-54 ft Geochemistry Samples #3 dtw = 53.72 bls after 15 hours								
63.5											Light brown to brown loosely to moderately consolidated finesand and silt with increased fines and water content
71											Tan to light brown, moderately to strongly consolidated fine sand/ siltstone
73.5											

MW-4

GEOLOGIC BORING/WELL LOG

Project #:	Project Name: Pojoaque ASR	Boring/Well #: MW-4
Geologist:	Driller/Company:	
Drilling Equip.:	Date Start:	Date Completed:
Surface Elev.:	Top of Casing Elev.:	Total Depth: / Well Depth:

DRILLING	SAMPLE								GEOLOGIC LOG		
				Blow Count							
Depth	PID Reading (ppm)	Sample Type	Sample ID	0-6"	6-12"	12-18"	18-24"	Recovery-(in)	USCS Class	Contact-Depth	Descriptions and Comments
73.5											Light brown to brown loosely to moderately consolidated fine sand and silt with increased clay content. Core sections are saturated and auger cuttings are soupy, silty, mud and clay. Increasing sand and gravel content with flowing water. Material flowed 2-3 ft into auger flight upon core barrel removal.
			74-75 ft. Geochemistry Sample Zone #4								
85											
			86-87 ft Geochemistry Sample Zone #5								
88.5 TD											

Water: Drinking Water Contaminants

Drinking Water Contaminants

National Primary Drinking Water Regulations

On this Page

- National Primary Drinking Water Regulations
- List of Drinking Water Contaminants and (MCLs)
- National Secondary Drinking Water Regulations
- List of Secondary Drinking Water Regulations
- Unregulated Contaminants

National Primary Drinking Water Regulations (NPDWRs or primary standards) are legally enforceable standards that apply to public water systems. Primary standards protect public health by limiting the levels of contaminants in drinking water. Visit the list of regulated contaminants with links for more details.

- List of Contaminants and their Maximum Contaminant Levels (MCLs)
- Regulation Development
- EPA's Regulated Contaminant Timeline (PDF) (1 pp, 86 K) (About PDF)
- National Primary Drinking Water Regulations- The complete regulations regarding these contaminants is available from the Code of Federal Regulations Website

List of Contaminants and their (MCLs)

Information on this section

- Alphabetical List (PDF) (6 pp, 924 K) (About PDF) EPA 816-F-09-0004, May 2009

An alphabetical listing with links to fact sheets on the primary drinking water regulations.

- Microorganisms
- Disinfectants
- Disinfection Byproducts
- Inorganic Chemicals
- Organic Chemicals
- Radionuclides

Microorganisms

Contaminant	MCLG[1] (mg/L)[2]	MCL or TT[1] (mg/L)[2]	Potential Health Effects from Long-Term Exposure Above the MCL (unless specified as short-term)	Sources of Contaminant in Drinking Water
Cryptosporidium	zero	TT[3]	Gastrointestinal illness (such as diarrhea, vomiting, and cramps)	Human and animal fecal waste
Giardia lamblia	zero	TT[3]	Gastrointestinal illness (such as diarrhea, vomiting, and cramps)	Human and animal fecal waste
Heterotrophic plate count (HPC)	n/a	TT[3]	HPC has no health effects; it is an analytic method used to measure the variety of bacteria that are common in water. The lower the concentration of bacteria in drinking water, the better maintained the water system is.	HPC measures a range of bacteria that are naturally present in the environment
Legionella	zero	TT[3]	Legionnaire's Disease, a type of pneumonia	Found naturally in water; multiplies in heating systems
Total Coliforms (including fecal coliform and *E. Coli*)	zero	5.0%[4]	Not a health threat in itself; it is used to indicate whether other potentially harmful bacteria may be present[5]	Coliforms are naturally present in the environment; as well as feces; fecal coliforms and *E. coli* only come from human and animal fecal waste.
Turbidity	n/a	TT[3]	Turbidity is a measure of the cloudiness of water. It is used to indicate water quality and filtration effectiveness (such as whether disease-causing organisms are present). Higher turbidity levels are	Soil runoff

			often associated with higher levels of disease-causing microorganisms such as viruses, parasites and some bacteria. These organisms can cause symptoms such as nausea, cramps, diarrhea, and associated headaches.	
Viruses (enteric)	zero	TT[3]	Gastrointestinal illness (such as diarrhea, vomiting, and cramps)	Human and animal fecal waste

Disinfection Byproducts

Contaminant	MCLG[1] (mg/L)[2]	MCL or TT[1] (mg/L)[2]	Potential Health Effects from Long-Term Exposure Above the MCL (unless specified as short-term)	Sources of Contaminant in Drinking Water
Bromate	zero	0.010	Increased risk of cancer	Byproduct of drinking water disinfection
Chlorite	0.8	1.0	Anemia; infants and young children: nervous system effects	Byproduct of drinking water disinfection
Haloacetic acids (HAA5)	n/a[6]	0.060[7]	Increased risk of cancer	Byproduct of drinking water disinfection
Total Trihalomethanes (TTHMs)	--> n/a[6]	--> 0.080[7]	Liver, kidney or central nervous system problems; increased risk of cancer	Byproduct of drinking water disinfection

Disinfectants

Contaminant	MCLG[1] (mg/L)[2]	MCL or TT[1] (mg/L)[2]	Potential Health Effects from Long-Term Exposure Above the MCL (unless specified as short-term)	Sources of Contaminant in Drinking Water
Chloramines (as Cl_2)	MRDLG=4[1]	MRDL=4.0[1]	Eye/nose irritation; stomach discomfort, anemia	Water additive used to control microbes
Chlorine (as Cl_2)	MRDLG=4[1]	MRDL=4.0[1]	Eye/nose irritation; stomach discomfort	Water additive used to control microbes
Chlorine dioxide (as ClO_2)	MRDLG=0.8[1]	MRDL=0.8[1]	Anemia; infants and young children: nervous system effects	Water additive used to control microbes

Inorganic Chemicals

Contaminant	MCLG[1] (mg/L)[2]	MCL or TT[1] (mg/L)[2]	Potential Health Effects from Long-Term Exposure Above the MCL (unless specified as short-term)	Sources of Contaminant in Drinking Water
Antimony	0.006	0.006	Increase in blood cholesterol; decrease in blood sugar	Discharge from petroleum refineries; fire retardants; ceramics; electronics; solder
Arsenic	0	0.010 as of 01/23/06	Skin damage or problems with circulatory systems, and may have increased risk of getting cancer	Erosion of natural deposits; runoff from orchards, runoff from glass and electronicsproduction wastes
Asbestos (fiber > 10 micrometers)	7 million fibers per liter (MFL)	7 MFL	Increased risk of developing benign intestinal polyps	Decay of asbestos cement in water mains; erosion of natural deposits
Barium	2	2	Increase in blood pressure	Discharge of drilling wastes; discharge from metal refineries; erosion of natural deposits

Beryllium	0.004	0.004	Intestinal lesions	Discharge from metal refineries and coal-burning factories; discharge from electrical, aerospace, and defense industries
Cadmium	0.005	0.005	Kidney damage	Corrosion of galvanized pipes; erosion of natural deposits; discharge from metal refineries; runoff from waste batteries and paints
Chromium (total)	0.1	0.1	Allergic dermatitis	Discharge from steel and pulp mills; erosion of natural deposits
Copper	1.3	TT[7]; Action Level=1.3	Short term exposure: Gastrointestinal distress Long term exposure: Liver or kidney damage People with Wilson's Disease should consult their personal doctor if the amount of copper in their water exceeds the action level	Corrosion of household plumbing systems; erosion of natural deposits
Cyanide (as free cyanide)	0.2	0.2	Nerve damage or thyroid problems	Discharge from steel/metal factories; discharge from plastic and fertilizer factories
Fluoride	4.0	4.0	Bone disease (pain and tenderness of the bones); Children may get mottled teeth	Water additive which promotes strong teeth; erosion of natural deposits; discharge from fertilizer and aluminum factories
Lead	zero	TT[7]; Action Level=0.015	Infants and children: Delays in physical or mental development; children could show slight deficits in attention span and learning abilities Adults: Kidney problems; high blood pressure	Corrosion of household plumbing systems; erosion of natural deposits
Mercury (inorganic)	0.002	0.002	Kidney damage	Erosion of natural deposits; discharge from refineries and factories; runoff from landfills and croplands
Nitrate (measured as Nitrogen)	10	10	Infants below the age of six months who drink water containing nitrate in excess of the MCL could become seriously ill and, if untreated, may die. Symptoms include shortness of breath and blue-baby syndrome.	Runoff from fertilizer use; leaking from septic tanks, sewage; erosion of natural deposits
Nitrite (measured as Nitrogen)	1	1	Infants below the age of six months who drink water containing nitrite in excess of the MCL could become seriously ill and, if untreated, may die. Symptoms include shortness of breath and blue-baby syndrome.	Runoff from fertilizer use; leaking from septic tanks, sewage; erosion of natural deposits
Selenium	0.05	0.05	Hair or fingernail loss; numbness in fingers or toes; circulatory problems	Discharge from petroleum refineries; erosion of natural deposits; discharge from mines
Thallium	0.0005	0.002	Hair loss; changes in blood; kidney, intestine, or liver problems	Leaching from ore-processing

				sites; discharge from electronics, glass, and drug factories

Organic Chemicals

Contaminant	MCLG[1] (mg/L)[2]	MCL or TT[1] (mg/L)[2]	Potential Health Effects from Long-Term Exposure Above the MCL (unless specified as short-term)	Sources of Contaminant in Drinking Water
Acrylamide	zero	TT[8]	Nervous system or blood problems; increased risk of cancer	Added to water during sewage/wastewater treatment
Alachlor	zero	0.002	Eye, liver, kidney or spleen problems; anemia; increased risk of cancer	Runoff from herbicide used on row crops
Atrazine	0.003	0.003	Cardiovascular system or reproductive problems	Runoff from herbicide used on row crops
Benzene	zero	0.005	Anemia; decrease in blood platelets; increased risk of cancer	Discharge from factories; leaching from gas storage tanks and landfills
Benzo(a)pyrene (PAHs)	zero	0.0002	Reproductive difficulties; increased risk of cancer	Leaching from linings of water storage tanks and distribution lines
Carbofuran	0.04	0.04	Problems with blood, nervous system, or reproductive system	Leaching of soil fumigant used on rice and alfalfa
Carbon tetrachloride	zero	0.005	Liver problems; increased risk of cancer	Discharge from chemical plants and other industrial activities
Chlordane	zero	0.002	Liver or nervous system problems; increased risk of cancer	Residue of banned termiticide
Chlorobenzene	0.1	0.1	Liver or kidney problems	Discharge from chemical and agricultural chemical factories
2,4-D	0.07	0.07	Kidney, liver, or adrenal gland problems	Runoff from herbicide used on row crops
Dalapon	0.2	0.2	Minor kidney changes	Runoff from herbicide used on rights of way
1,2-Dibromo-3-chloropropane (DBCP)	zero	0.0002	Reproductive difficulties; increased risk of cancer	Runoff/leaching from soil fumigant used on soybeans, cotton, pineapples, and orchards
o-Dichlorobenzene	0.6	0.6	Liver, kidney, or circulatory system problems	Discharge from industrial chemical factories
p-Dichlorobenzene	0.075	0.075	Anemia; liver, kidney or spleen damage; changes in blood	Discharge from industrial chemical factories
1,2-Dichloroethane	zero	0.005	Increased risk of cancer	Discharge from industrial chemical factories
1,1-Dichloroethylene	0.007	0.007	Liver problems	Discharge from industrial chemical factories
cis-1,2-Dichloroethylene	0.07	0.07	Liver problems	Discharge from industrial chemical factories
trans-1,2-Dichloroethylene	0.1	0.1	Liver problems	Discharge from industrial chemical factories

Dichloromethane	zero	0.005	Liver problems; increased risk of cancer	Discharge from drug and chemical factories
1,2-Dichloropropane	zero	0.005	Increased risk of cancer	Discharge from industrial chemical factories
Di(2-ethylhexyl) adipate	0.4	0.4	Weight loss, liver problems, or possible reproductive difficulties.	Discharge from chemical factories
Di(2-ethylhexyl) phthalate	zero	0.006	Reproductive difficulties; liver problems; increased risk of cancer	Discharge from rubber and chemical factories
Dinoseb	0.007	0.007	Reproductive difficulties	Runoff from herbicide used on soybeans and vegetables
Dioxin (2,3,7,8-TCDD)	zero	0.00000003	Reproductive difficulties; increased risk of cancer	Emissions from waste incineration and other combustion; discharge from chemical factories
Diquat	0.02	0.02	Cataracts	Runoff from herbicide use
Endothall	0.1	0.1	Stomach and intestinal problems	Runoff from herbicide use
Endrin	0.002	0.002	Liver problems	Residue of banned insecticide
Epichlorohydrin	zero	TT[8]	Increased cancer risk, and over a long period of time, stomach problems	Discharge from industrial chemical factories; an impurity of some water treatment chemicals
Ethylbenzene	0.7	0.7	Liver or kidneys problems	Discharge from petroleum refineries
Ethylene dibromide	zero	0.00005	Problems with liver, stomach, reproductive system, or kidneys; increased risk of cancer	Discharge from petroleum refineries
Glyphosate	0.7	0.7	Kidney problems; reproductive difficulties	Runoff from herbicide use
Heptachlor	zero	0.0004	Liver damage; increased risk of cancer	Residue of banned termiticide
Heptachlor epoxide	zero	0.0002	Liver damage; increased risk of cancer	Breakdown of heptachlor
Hexachlorobenzene	zero	0.001	Liver or kidney problems; reproductive difficulties; increased risk of cancer	Discharge from metal refineries and agricultural chemical factories
Hexachlorocyclopentadiene	0.05	0.05	Kidney or stomach problems	Discharge from chemical factories
Lindane	0.0002	0.0002	Liver or kidney problems	Runoff/leaching from insecticide used on cattle, lumber, gardens
Methoxychlor	0.04	0.04	Reproductive difficulties	Runoff/leaching from insecticide used on fruits, vegetables, alfalfa, livestock
Oxamyl (Vydate)	0.2	0.2	Slight nervous system effects	Runoff/leaching from insecticide used on apples, potatoes, and tomatoes
Polychlorinated biphenyls (PCBs)	zero	0.0005	Skin changes; thymus gland problems; immune deficiencies; reproductive or nervous system difficulties; increased risk of cancer	Runoff from landfills; discharge of waste chemicals

Pentachlorophenol	zero	0.001	Liver or kidney problems; increased cancer risk	Discharge from wood preserving factories
Picloram	0.5	0.5	Liver problems	Herbicide runoff
Simazine	0.004	0.004	Problems with blood	Herbicide runoff
Styrene	0.1	0.1	Liver, kidney, or circulatory system problems	Discharge from rubber and plastic factories; leaching from landfills
Tetrachloroethylene	zero	0.005	Liver problems; increased risk of cancer	Discharge from factories and dry cleaners
Toluene	1	1	Nervous system, kidney, or liver problems	Discharge from petroleum factories
Toxaphene	zero	0.003	Kidney, liver, or thyroid problems; increased risk of cancer	Runoff/leaching from insecticide used on cotton and cattle
2,4,5-TP (**Silvex**)	0.05	0.05	Liver problems	Residue of banned herbicide
1,2,4-Trichlorobenzene	0.07	0.07	Changes in adrenal glands	Discharge from textile finishing factories
1,1,1-Trichloroethane	0.20	0.2	Liver, nervous system, or circulatory problems	Discharge from metal degreasing sites and other factories
1,1,2-Trichloroethane	0.003	0.005	Liver, kidney, or immune system problems	Discharge from industrial chemical factories
Trichloroethylene	zero	0.005	Liver problems; increased risk of cancer	Discharge from metal degreasing sites and other factories
Vinyl chloride	zero	0.002	Increased risk of cancer	Leaching from PVC pipes; discharge from plastic factories
Xylenes (total)	10	10	Nervous system damage	Discharge from petroleum factories; discharge from chemical factories

Radionuclides

Contaminant	MCLG[1] (MG/L)[2]	MCL or TT[1] (MG/L)[2]	Potential Health Effects from Long-Term Exposure Above the MCL (unless specified as short-term)	Sources of Contaminant in Drinking Water
Alpha particles	none[7] ---------- zero	15 picocuries per Liter (PCI/L)	Increased risk of cancer	Erosion of natural deposits of certain minerals that are radioactive and may emit a form of radiation known as alpha radiation
Beta particles and photon emitters	none[7] ---------- zero	4 millirems per year	Increased risk of cancer	Decay of natural and man-made deposits of certain minerals that are radioactive and may emit forms of radiation known as photons and beta radiation
Radium 226 and Radium 228 (combined)	none[7] ---------- zero	5 PCI/L	Increased risk of cancer	Erosion of natural deposits
Uranium	zero	30 UG/L as of 12/08/03	Increased risk of cancer, kidney toxicity	Erosion of natural deposits

Notes

[1] **Definitions:**

- Maximum Contaminant Level Goal (MCLG) - The level of a contaminant in drinking water below which there is no known or expected risk to health. MCLGs allow for a margin of safety and are non-enforceable public health goals.
- Maximum Contaminant Level (MCL) - The highest level of a contaminant that is allowed in drinking water. MCLs are set as close to MCLGs as feasible using the best available treatment technology and taking cost into consideration. MCLs are enforceable standards.
- Maximum Residual Disinfectant Level Goal (MRDLG) - The level of a drinking water disinfectant below which there is no known or expected risk to health. MRDLGs do not reflect the benefits of the use of disinfectants to control microbial contaminants.)
- Treatment Technique (TT) - A required process intended to reduce the level of a contaminant in drinking water.
- Maximum Residual Disinfectant Level (MRDL) - The highest level of a disinfectant allowed in drinking water. There is convincing evidence that addition of a disinfectant is necessary for control of microbial contaminants.
- [2] Units are in milligrams per liter (MG/L) unless otherwise noted. Milligrams per liter are equivalent to parts per million (PPM).
  [3] EPA's surface water treatment rules require systems using surface water or ground water under the direct influence of surface water to

  (1) disinfect their water, and
  (2) filter their water or
  meet criteria for avoiding filtration so that the following contaminants are controlled at the following levels:
  - *Cryptosporidium*: Unfiltered systems are required to include *Cryptosporidium* in their existing watershed control provisions
  - *Giardia lamblia*: 99.9% removal/inactivation.
  - Viruses: 99.99% removal/inactivation.
  - *Legionella*: No limit, but EPA believes that if *Giardia* and viruses are removed/inactivated, according to the treatment techniques in the Surface Water Treatment Rule, *Legionella* will also be controlled.
  - Turbidity: For systems that use conventional or direct filtration, at no time can turbidity (cloudiness of water) go higher than 1 Nephelometric Turbidity Unit (NTU), and samples for turbidity must be less than or equal to 0.3 NTUs in at least 95 percent of the samples in any month. Systems that use filtration other than the conventional or direct filtration must follow state limits, which must include turbidity at no time exceeding 5 NTUs.
  - Heterotrophic Plate Count (HPC): No more than 500 bacterial colonies per milliliter.
  - Long Term 1 Enhanced Surface Water Treatment: Surface water systems or groundwater under the direct influence (GWUDI) systems serving fewer than 10,000 people must comply with the applicable Long Term 1 Enhanced Surface Water Treatment Rule provisions (such as turbidity standards, individual filter monitoring, *Cryptosporidium* removal requirements, updated watershed control requirements for unfiltered systems).
  - Long Term 2 Enhanced Surface Water Treatment Rule: This rule applies to all surface water systems or ground water systems under the direct influence of surface water. The rule targets additional *Cryptosporidium* treatment requirements for higher risk systems and includes provisions to reduce risks from uncovered finished water storage facilities and to ensure that the systems maintain microbial protection as they take steps to reduce the formation of disinfection byproducts.
  - Filter Backwash Recycling: The Filter Backwash Recycling Rule requires systems that recycle to return specific recycle flows through all processes of the system's existing conventional or direct filtration system or at an alternate location approved by the state.

[4] No more than 5.0% samples total coliform-positive (TC-POSITIVE) in a month. (For water systems that collect fewer than 40 routine samples per month, no more than one sample can be total coliform-positive per month.) Every sample that has total coliform must be analyzed for either fecal coliforms or *E. coli* if two consecutive TC-POSITIVE samples, and one is also positive for *E.coli* fecal coliforms, system has an acute MCL violation.
[5] Fecal coliform and *E. coli* are bacteria whose presence indicates that the water may be contaminated with human or animal wastes. Disease-causing microbes (pathogens) in these wastes can cause diarrhea, cramps, nausea, headaches, or other symptoms. These pathogens may pose a special health risk for infants, young children, and people with severely compromised immune systems.

[6] Although there is no collective MCLG for this contaminant group, there are individual MCLGs for some of the individual contaminants:

- Trihalomethanes: bromodichloromethane (zero); bromoform (zero); dibromochloromethane (0.06 MG/L): chloroform (0.07 MG/L.
- Haloacetic acids: dichloroacetic acid (zero); trichloroacetic acid (0.02 MG/L); monochloroacetic acid (0.07 MG/L). Bromoacetic acid and dibromoacetic acid are regulated with this group but have no MCLGs.

[7] Lead and copper are regulated by a treatment technique that requires systems to control the corrosiveness of their water. If more than 10% of tap water samples exceed the action level, water systems must take additional steps. For copper, the action level is 1.3 MG/L, and for lead is 0.015 MG/L.

[8] Each water system must certify, in writing, to the state (using third-party or manufacturer's certification) that when acrylamide and epichlorohydrin are used to treat water, the combination (or product) of dose and monomer level does not exceed the levels specified, as follows:

- Acrylamide = 0.05% dosed at 1 MG/L (or equivalent)
- Epichlorohydrin = 0.01% dosed at 20 MG/L (or equivalent)

National Secondary Drinking Water Regulations

National Secondary Drinking Water Regulations (NSDWRs or secondary standards) are non-enforceable guidelines regulating contaminants that may cause cosmetic effects (such as skin or tooth discoloration) or aesthetic effects (such as taste, odor, or color) in drinking water. EPA recommends secondary standards to water systems but does not require systems to comply. However, states may choose to adopt them as enforceable standards.

- National Secondary Drinking Water Regulations - The complete regulations regarding these contaminants is available from the Code of Federal Regulations Web Site.
- For more information, read Secondary Drinking Water Regulations: Guidance for Nuisance Chemicals.

List of National Secondary Drinking Water Regulations

Contaminant	Secondary Standard
Aluminum	0.05 to 0.2 MG/L
Chloride	250 MG/L
Color	15 (color units)
Copper	1.0 MG/L
Corrosivity	noncorrosive
Fluoride	2.0 MG/L
Foaming Agents	0.5 MG/L
Iron	0.3 MG/L
Manganese	0.05 MG/L
Odor	3 threshold odor number
PH	6.5-8.5
Silver	0.10 MG/L
Sulfate	250 MG/L
Total Dissolved Solids	500 MG/L
Zinc	5 MG/L

Unregulated Contaminants

This list of contaminants which, at the time of publication, are not subject to any proposed or promulgated national primary drinking water regulation (NSDWRs), are known or anticipated to occur in public water systems, and may require regulations under the Safe Drinking Water Act (SDWA). For more information check out the list, or visit the Drinking Water Contaminant Candidate List (CCL) website.

- Drinking Water Contaminant Candidate List (CCL) website
- Unregulated Contaminant Monitoring Program (UCM)
- Information on specific unregulated contaminants
  - MTBE (methyl-t-butyl ether) in drinking water

Last updated on Wednesday, October 29, 2014

```
   Input file: E:\Project Stuff\Models\Trace Metal_Inputst.pqi
  Output file: E:\Project Stuff\Models\Trace Metal_Inputst.pqo
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.1.2-8538\database
\wateq4f.dat

------------------
Reading data base.
------------------

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

      DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 3.1.2-8538\database
\wateq4f.dat
      TITLE Professional Project Geochemical Model
      SOLUTION   MW-3
              units   ppm
              pH      7.69
              temp    15.6
              O(0)            4.21
              Ca              49.33
              Mg              4.69
              Na              36.6
              K               3.76
              Ba              0.0623
              Cd              0.00038
              Cu              0
              Zn              0.0413
              Pb              0.000234
              Mn              0.0051
              Se              0.00442
              Ni              0.00142
              Fe              0.00862
              Al              0.0748
              U               0.0234
              As              0.00302
              Cl              19
              Alkalinity      155.7 as HCO3
              S(6)            51.8
              Si              26.9
      END
-----
TITLE
-----

 Professional Project Geochemical Model

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

Initial solution 1.     MW-3

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

      Elements           Molality       Moles

      Al                2.773e-06   2.773e-06
```

Alkalinity	2.553e-03	2.553e-03
As	4.032e-08	4.032e-08
Ba	4.538e-07	4.538e-07
Ca	1.231e-03	1.231e-03
Cd	3.382e-09	3.382e-09
Cl	5.361e-04	5.361e-04
Fe	1.544e-07	1.544e-07
K	9.619e-05	9.619e-05
Mg	1.930e-04	1.930e-04
Mn	9.286e-08	9.286e-08
Na	1.593e-03	1.593e-03
Ni	2.420e-08	2.420e-08
O(0)	2.632e-04	2.632e-04
Pb	1.130e-09	1.130e-09
S(6)	5.394e-04	5.394e-04
Se	5.600e-08	5.600e-08
Si	4.479e-04	4.479e-04
U	9.834e-08	9.834e-08
Zn	6.320e-07	6.320e-07

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

pH	= 7.690
pe	= 4.000
Activity of water	= 1.000
Ionic strength	= 5.998e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 2.648e-03
Total CO2 (mol/kg)	= 2.648e-03
Temperature (°C)	= 15.60
Electrical balance (eq)	= 3.806e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 4.55
Iterations	= 11
Total H	= 1.110167e+02
Total O	= 5.551826e+01

----------Redox couples----------

Redox couple	pe	Eh (volts)
O(-2)/O(0)	13.6641	0.7828

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	2.520e-07	2.321e-07	-6.599	-6.634	-0.036	(0)
H+	2.196e-08	2.042e-08	-7.658	-7.690	-0.032	0.00
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.03
Al	2.773e-06					
Al(OH)4-	2.733e-06	2.522e-06	-5.563	-5.598	-0.035	(0)
Al(OH)3	3.021e-08	3.026e-08	-7.520	-7.519	0.001	(0)
Al(OH)2+	9.487e-09	8.768e-09	-8.023	-8.057	-0.034	(0)
AlOH+2	7.460e-11	5.444e-11	-10.127	-10.264	-0.137	(0)
Al+3	4.026e-13	2.089e-13	-12.395	-12.680	-0.285	(0)
AlSO4+	2.182e-13	2.014e-13	-12.661	-12.696	-0.035	(0)
Al(SO4)2-	2.281e-15	2.105e-15	-14.642	-14.677	-0.035	(0)
AlHSO4+2	4.695e-22	3.395e-22	-21.328	-21.469	-0.141	(0)
As(3)	1.323e-17					
H3AsO3	1.289e-17	1.291e-17	-16.890	-16.889	0.001	(0)
H2AsO3-	3.381e-19	3.118e-19	-18.471	-18.506	-0.035	(0)
H4AsO3+	1.416e-25	1.306e-25	-24.849	-24.884	-0.035	(0)
HAsO3-2	2.772e-26	2.005e-26	-25.557	-25.698	-0.141	(0)
AsO3-3	2.914e-34	1.405e-34	-33.536	-33.852	-0.317	(0)
As(5)	4.032e-08					
HAsO4-2	3.248e-08	2.349e-08	-7.488	-7.629	-0.141	(0)
H2AsO4-	7.841e-09	7.231e-09	-8.106	-8.141	-0.035	(0)

AsO4-3	4.205e-12	2.028e-12	-11.376	-11.693	-0.317	(0)
H3AsO4	2.681e-14	2.685e-14	-13.572	-13.571	0.001	(0)
Ba	4.538e-07					
Ba+2	3.980e-07	2.896e-07	-6.400	-6.538	-0.138	(0)
BaSO4	5.011e-08	5.018e-08	-7.300	-7.299	0.001	(0)
BaHCO3+	5.146e-09	4.746e-09	-8.289	-8.324	-0.035	(0)
BaCO3	5.273e-10	5.280e-10	-9.278	-9.277	0.001	(0)
BaOH+	5.203e-13	4.805e-13	-12.284	-12.318	-0.035	(0)
C(4)	2.648e-03					
HCO3-	2.487e-03	2.298e-03	-2.604	-2.639	-0.034	(0)
CO2	1.216e-04	1.217e-04	-3.915	-3.915	0.001	(0)
CaHCO3+	2.231e-05	2.064e-05	-4.652	-4.685	-0.034	(0)
CO3-2	5.841e-06	4.262e-06	-5.234	-5.370	-0.137	(0)
CaCO3	5.132e-06	5.139e-06	-5.290	-5.289	0.001	(0)
MgHCO3+	3.731e-06	3.440e-06	-5.428	-5.463	-0.035	(0)
NaHCO3	1.891e-06	1.894e-06	-5.723	-5.723	0.001	(0)
MgCO3	4.645e-07	4.652e-07	-6.333	-6.332	0.001	(0)
ZnCO3	1.938e-07	1.940e-07	-6.713	-6.712	0.001	(0)
NaCO3-	7.713e-08	7.129e-08	-7.113	-7.147	-0.034	(0)
ZnHCO3+	7.158e-08	6.601e-08	-7.145	-7.180	-0.035	(0)
UO2(CO3)3-4	4.916e-08	1.344e-08	-7.308	-7.872	-0.563	(0)
UO2(CO3)2-2	4.856e-08	3.512e-08	-7.314	-7.454	-0.141	(0)
Zn(CO3)2-2	2.445e-08	1.768e-08	-7.612	-7.752	-0.141	(0)
NiCO3	2.267e-08	2.270e-08	-7.644	-7.644	0.001	(0)
MnCO3	1.587e-08	1.589e-08	-7.799	-7.799	0.001	(0)
MnHCO3+	1.041e-08	9.614e-09	-7.983	-8.017	-0.035	(0)
BaHCO3+	5.146e-09	4.746e-09	-8.289	-8.324	-0.035	(0)
FeHCO3+	4.943e-09	4.558e-09	-8.306	-8.341	-0.035	(0)
FeCO3	2.025e-09	2.028e-09	-8.694	-8.693	0.001	(0)
PbCO3	1.049e-09	1.050e-09	-8.979	-8.979	0.001	(0)
BaCO3	5.273e-10	5.280e-10	-9.278	-9.277	0.001	(0)
UO2CO3	4.189e-10	4.195e-10	-9.378	-9.377	0.001	(0)
NiHCO3+	2.472e-10	2.280e-10	-9.607	-9.642	-0.035	(0)
Ni(CO3)2-2	2.326e-10	1.682e-10	-9.633	-9.774	-0.141	(0)
CdHCO3+	1.653e-10	1.525e-10	-9.782	-9.817	-0.035	(0)
PbHCO3+	2.807e-11	2.588e-11	-10.552	-10.587	-0.035	(0)
Pb(CO3)2-2	1.555e-11	1.124e-11	-10.808	-10.949	-0.141	(0)
CdCO3	7.093e-12	7.103e-12	-11.149	-11.149	0.001	(0)
Cd(CO3)2-2	1.324e-13	9.574e-14	-12.878	-13.019	-0.141	(0)
(UO2)3(CO3)6-6	1.659e-18	8.974e-20	-17.780	-19.047	-1.267	(0)
UO2(CO3)3-5	1.202e-24	1.585e-25	-23.920	-24.800	-0.880	(0)
U(CO3)4-4	2.986e-31	8.165e-32	-30.525	-31.088	-0.563	(0)
U(CO3)5-6	2.700e-35	1.460e-36	-34.569	-35.836	-1.267	(0)
Ca	1.231e-03					
Ca+2	1.151e-03	8.394e-04	-2.939	-3.076	-0.137	(0)
CaSO4	5.281e-05	5.289e-05	-4.277	-4.277	0.001	(0)
CaHCO3+	2.231e-05	2.064e-05	-4.652	-4.685	-0.034	(0)
CaCO3	5.132e-06	5.139e-06	-5.290	-5.289	0.001	(0)
CaOH+	7.373e-09	6.822e-09	-8.132	-8.166	-0.034	(0)
CaHSO4+	6.168e-12	5.688e-12	-11.210	-11.245	-0.035	(0)
Cd	3.382e-09					
Cd+2	2.901e-09	2.098e-09	-8.537	-8.678	-0.141	(0)
CdSO4	1.969e-10	1.972e-10	-9.706	-9.705	0.001	(0)
CdHCO3+	1.653e-10	1.525e-10	-9.782	-9.817	-0.035	(0)
CdCl+	1.039e-10	9.580e-11	-9.983	-10.019	-0.035	(0)
CdCO3	7.093e-12	7.103e-12	-11.149	-11.149	0.001	(0)
CdOH+	4.512e-12	4.161e-12	-11.346	-11.381	-0.035	(0)
CdOHCl	1.573e-12	1.576e-12	-11.803	-11.803	0.001	(0)
Cd(SO4)2-2	1.097e-12	7.931e-13	-11.960	-12.101	-0.141	(0)
CdCl2	1.900e-13	1.903e-13	-12.721	-12.721	0.001	(0)
Cd(CO3)2-2	1.324e-13	9.574e-14	-12.878	-13.019	-0.141	(0)
Cd(OH)2	2.244e-14	2.248e-14	-13.649	-13.648	0.001	(0)
CdCl3-	5.556e-17	5.124e-17	-16.255	-16.290	-0.035	(0)
Cd(OH)3-	1.339e-19	1.235e-19	-18.873	-18.908	-0.035	(0)
Cd2OH+3	1.000e-19	4.825e-20	-19.000	-19.317	-0.317	(0)
Cd(OH)4-2	7.454e-26	5.390e-26	-25.128	-25.268	-0.141	(0)
Cl	5.361e-04					
Cl-	5.361e-04	4.939e-04	-3.271	-3.306	-0.036	(0)

ZnCl+	2.144e-10	1.977e-10	-9.669	-9.704	-0.035	(0)
ZnOHCl	1.825e-10	1.827e-10	-9.739	-9.738	0.001	(0)
CdCl+	1.039e-10	9.580e-11	-9.983	-10.019	-0.035	(0)
MnCl+	1.023e-10	9.444e-11	-9.990	-10.025	-0.035	(0)
FeCl+	1.464e-11	1.352e-11	-10.834	-10.869	-0.035	(0)
CdOHCl	1.573e-12	1.576e-12	-11.803	-11.803	0.001	(0)
NiCl+	9.667e-13	8.914e-13	-12.015	-12.050	-0.035	(0)
PbCl+	2.376e-13	2.191e-13	-12.624	-12.659	-0.035	(0)
CdCl2	1.900e-13	1.903e-13	-12.721	-12.721	0.001	(0)
ZnCl2	9.818e-14	9.832e-14	-13.008	-13.007	0.001	(0)
MnCl2	2.033e-14	2.036e-14	-13.692	-13.691	0.001	(0)
NiCl2	1.596e-15	1.598e-15	-14.797	-14.796	0.001	(0)
PbCl2	2.053e-16	2.056e-16	-15.688	-15.687	0.001	(0)
ZnCl3-	5.575e-17	5.140e-17	-16.254	-16.289	-0.035	(0)
CdCl3-	5.556e-17	5.124e-17	-16.255	-16.290	-0.035	(0)
UO2Cl+	1.759e-17	1.622e-17	-16.755	-16.790	-0.035	(0)
MnCl3-	2.998e-18	2.769e-18	-17.523	-17.558	-0.035	(0)
FeCl+2	1.677e-19	1.220e-19	-18.775	-18.914	-0.138	(0)
PbCl3-	8.239e-20	7.597e-20	-19.084	-19.119	-0.035	(0)
ZnCl4-2	1.619e-20	1.178e-20	-19.791	-19.929	-0.138	(0)
FeCl2+	3.971e-22	3.662e-22	-21.401	-21.436	-0.035	(0)
UO2Cl2	3.912e-22	3.918e-22	-21.408	-21.407	0.001	(0)
PbCl4-2	2.305e-23	1.667e-23	-22.637	-22.778	-0.141	(0)
FeCl3	1.806e-26	1.808e-26	-25.743	-25.743	0.001	(0)
UCl+3	0.000e+00	0.000e+00	-43.668	-43.985	-0.317	(0)
Fe(2)	3.523e-08					
Fe+2	2.707e-08	1.983e-08	-7.568	-7.703	-0.135	(0)
FeHCO3+	4.943e-09	4.558e-09	-8.306	-8.341	-0.035	(0)
FeCO3	2.025e-09	2.028e-09	-8.694	-8.693	0.001	(0)
FeSO4	1.020e-09	1.021e-09	-8.991	-8.991	0.001	(0)
FeOH+	1.610e-10	1.487e-10	-9.793	-9.828	-0.035	(0)
FeCl+	1.464e-11	1.352e-11	-10.834	-10.869	-0.035	(0)
Fe(OH)2	2.661e-14	2.665e-14	-13.575	-13.574	0.001	(0)
FeHSO4+	1.458e-16	1.344e-16	-15.836	-15.872	-0.035	(0)
Fe(OH)3-	4.773e-17	4.408e-17	-16.321	-16.356	-0.035	(0)
Fe(3)	1.192e-07					
Fe(OH)3	9.203e-08	9.215e-08	-7.036	-7.035	0.001	(0)
Fe(OH)2+	2.413e-08	2.230e-08	-7.617	-7.652	-0.034	(0)
Fe(OH)4-	3.015e-09	2.786e-09	-8.521	-8.555	-0.034	(0)
FeOH+2	2.731e-12	1.987e-12	-11.564	-11.702	-0.138	(0)
FeSO4+	3.685e-17	3.403e-17	-16.434	-16.468	-0.035	(0)
Fe+3	2.145e-17	1.113e-17	-16.668	-16.954	-0.285	(0)
Fe(SO4)2-	2.688e-19	2.479e-19	-18.571	-18.606	-0.035	(0)
FeCl+2	1.677e-19	1.220e-19	-18.775	-18.914	-0.138	(0)
Fe2(OH)2+4	5.804e-22	1.587e-22	-21.236	-21.799	-0.563	(0)
FeCl2+	3.971e-22	3.662e-22	-21.401	-21.436	-0.035	(0)
FeHSO4+2	2.620e-24	1.894e-24	-23.582	-23.723	-0.141	(0)
FeCl3	1.806e-26	1.808e-26	-25.743	-25.743	0.001	(0)
Fe3(OH)4+5	1.373e-26	1.811e-27	-25.862	-26.742	-0.880	(0)
H(0)	6.492e-27					
H2	3.246e-27	3.251e-27	-26.489	-26.488	0.001	(0)
K	9.619e-05					
K+	9.600e-05	8.843e-05	-4.018	-4.053	-0.036	(0)
KSO4-	1.962e-07	1.814e-07	-6.707	-6.741	-0.034	(0)
Mg	1.930e-04					
Mg+2	1.804e-04	1.321e-04	-3.744	-3.879	-0.135	(0)
MgSO4	8.329e-06	8.340e-06	-5.079	-5.079	0.001	(0)
MgHCO3+	3.731e-06	3.440e-06	-5.428	-5.463	-0.035	(0)
MgCO3	4.645e-07	4.652e-07	-6.333	-6.332	0.001	(0)
MgOH+	1.056e-08	9.779e-09	-7.976	-8.010	-0.033	(0)
Mn(2)	9.286e-08					
Mn+2	6.406e-08	4.694e-08	-7.193	-7.328	-0.135	(0)
MnCO3	1.587e-08	1.589e-08	-7.799	-7.799	0.001	(0)
MnHCO3+	1.041e-08	9.614e-09	-7.983	-8.017	-0.035	(0)
MnSO4	2.395e-09	2.398e-09	-8.621	-8.620	0.001	(0)
MnCl+	1.023e-10	9.444e-11	-9.990	-10.025	-0.035	(0)
MnOH+	2.900e-11	2.678e-11	-10.538	-10.572	-0.035	(0)
MnCl2	2.033e-14	2.036e-14	-13.692	-13.691	0.001	(0)

MnCl3-	2.998e-18	2.769e-18	-17.523	-17.558	-0.035	(0)
Mn(OH)3-	9.460e-20	8.737e-20	-19.024	-19.059	-0.035	(0)
Mn(3)	6.776e-30					
Mn+3	6.776e-30	3.515e-30	-29.169	-29.454	-0.285	(0)
Mn(6)	0.000e+00					
MnO4-2	0.000e+00	0.000e+00	-51.690	-51.828	-0.138	(0)
Mn(7)	0.000e+00					
MnO4-	0.000e+00	0.000e+00	-57.811	-57.847	-0.036	(0)
Na	1.593e-03					
Na+	1.588e-03	1.466e-03	-2.799	-2.834	-0.035	(0)
NaSO4-	2.584e-06	2.388e-06	-5.588	-5.622	-0.034	(0)
NaHCO3	1.891e-06	1.894e-06	-5.723	-5.723	0.001	(0)
NaCO3-	7.713e-08	7.129e-08	-7.113	-7.147	-0.034	(0)
Ni	2.420e-08					
NiCO3	2.267e-08	2.270e-08	-7.644	-7.644	0.001	(0)
Ni+2	9.937e-10	7.186e-10	-9.003	-9.144	-0.141	(0)
NiHCO3+	2.472e-10	2.280e-10	-9.607	-9.642	-0.035	(0)
Ni(CO3)2-2	2.326e-10	1.682e-10	-9.633	-9.774	-0.141	(0)
NiSO4	4.450e-11	4.456e-11	-10.352	-10.351	0.001	(0)
NiOH+	2.662e-12	2.455e-12	-11.575	-11.610	-0.035	(0)
NiCl+	9.667e-13	8.914e-13	-12.015	-12.050	-0.035	(0)
Ni(OH)2	1.721e-13	1.723e-13	-12.764	-12.764	0.001	(0)
NiCl2	1.596e-15	1.598e-15	-14.797	-14.796	0.001	(0)
Ni(SO4)2-2	1.244e-15	8.995e-16	-14.905	-15.046	-0.141	(0)
Ni(OH)3-	9.152e-17	8.439e-17	-16.038	-16.074	-0.035	(0)
O(0)	2.632e-04					
O2	1.316e-04	1.318e-04	-3.881	-3.880	0.001	(0)
Pb	1.130e-09					
PbCO3	1.049e-09	1.050e-09	-8.979	-8.979	0.001	(0)
PbHCO3+	2.807e-11	2.588e-11	-10.552	-10.587	-0.035	(0)
Pb+2	1.960e-11	1.418e-11	-10.708	-10.848	-0.141	(0)
Pb(CO3)2-2	1.555e-11	1.124e-11	-10.808	-10.949	-0.141	(0)
PbOH+	1.468e-11	1.354e-11	-10.833	-10.868	-0.035	(0)
PbSO4	2.753e-12	2.756e-12	-11.560	-11.560	0.001	(0)
Pb(OH)2	2.576e-13	2.579e-13	-12.589	-12.589	0.001	(0)
PbCl+	2.376e-13	2.191e-13	-12.624	-12.659	-0.035	(0)
Pb(SO4)2-2	6.916e-15	5.002e-15	-14.160	-14.301	-0.141	(0)
PbCl2	2.053e-16	2.056e-16	-15.688	-15.687	0.001	(0)
Pb(OH)3-	1.573e-16	1.450e-16	-15.803	-15.839	-0.035	(0)
PbCl3-	8.239e-20	7.597e-20	-19.084	-19.119	-0.035	(0)
Pb(OH)4-2	2.250e-20	1.627e-20	-19.648	-19.789	-0.141	(0)
Pb2OH+3	8.910e-21	4.296e-21	-20.050	-20.367	-0.317	(0)
PbCl4-2	2.305e-23	1.667e-23	-22.637	-22.778	-0.141	(0)
Pb3(OH)4+2	6.966e-27	5.037e-27	-26.157	-26.298	-0.141	(0)
S(6)	5.394e-04					
SO4-2	4.754e-04	3.458e-04	-3.323	-3.461	-0.138	(0)
CaSO4	5.281e-05	5.289e-05	-4.277	-4.277	0.001	(0)
MgSO4	8.329e-06	8.340e-06	-5.079	-5.079	0.001	(0)
NaSO4-	2.584e-06	2.388e-06	-5.588	-5.622	-0.034	(0)
KSO4-	1.962e-07	1.814e-07	-6.707	-6.741	-0.034	(0)
BaSO4	5.011e-08	5.018e-08	-7.300	-7.299	0.001	(0)
ZnSO4	1.714e-08	1.716e-08	-7.766	-7.765	0.001	(0)
MnSO4	2.395e-09	2.398e-09	-8.621	-8.620	0.001	(0)
FeSO4	1.020e-09	1.021e-09	-8.991	-8.991	0.001	(0)
HSO4-	6.108e-10	5.637e-10	-9.214	-9.249	-0.035	(0)
CdSO4	1.969e-10	1.972e-10	-9.706	-9.705	0.001	(0)
Zn(SO4)2-2	7.187e-11	5.197e-11	-10.143	-10.284	-0.141	(0)
NiSO4	4.450e-11	4.456e-11	-10.352	-10.351	0.001	(0)
CaHSO4+	6.168e-12	5.688e-12	-11.210	-11.245	-0.035	(0)
PbSO4	2.753e-12	2.756e-12	-11.560	-11.560	0.001	(0)
Cd(SO4)2-2	1.097e-12	7.931e-13	-11.960	-12.101	-0.141	(0)
AlSO4+	2.182e-13	2.014e-13	-12.661	-12.696	-0.035	(0)
UO2SO4	9.284e-15	9.297e-15	-14.032	-14.032	0.001	(0)
Pb(SO4)2-2	6.916e-15	5.002e-15	-14.160	-14.301	-0.141	(0)
Al(SO4)2-	2.281e-15	2.105e-15	-14.642	-14.677	-0.035	(0)
Ni(SO4)2-2	1.244e-15	8.995e-16	-14.905	-15.046	-0.141	(0)
FeHSO4+	1.458e-16	1.344e-16	-15.836	-15.872	-0.035	(0)
FeSO4+	3.685e-17	3.403e-17	-16.434	-16.468	-0.035	(0)

UO2(SO4)2-2	3.545e-17	2.563e-17	-16.450	-16.591	-0.141	(0)
Fe(SO4)2-	2.688e-19	2.479e-19	-18.571	-18.606	-0.035	(0)
AlHSO4+2	4.695e-22	3.395e-22	-21.328	-21.469	-0.141	(0)
FeHSO4+2	2.620e-24	1.894e-24	-23.582	-23.723	-0.141	(0)
U(SO4)2	7.659e-40	7.670e-40	-39.116	-39.115	0.001	(0)
USO4+2	5.100e-40	3.688e-40	-39.292	-39.433	-0.141	(0)
Se(-2)	0.000e+00					
HSe-	0.000e+00	0.000e+00	-43.456	-43.491	-0.035	(0)
H2Se	0.000e+00	0.000e+00	-47.255	-47.255	0.001	(0)
Se(4)	5.600e-08					
HSeO3-	4.676e-08	4.312e-08	-7.330	-7.365	-0.035	(0)
SeO3-2	9.236e-09	6.679e-09	-8.035	-8.175	-0.141	(0)
H2SeO3	4.944e-13	4.951e-13	-12.306	-12.305	0.001	(0)
Se(6)	1.229e-15					
SeO4-2	1.229e-15	8.885e-16	-14.911	-15.051	-0.141	(0)
HSeO4-	6.865e-22	6.331e-22	-21.163	-21.199	-0.035	(0)
Si	4.479e-04					
H4SiO4	4.454e-04	4.460e-04	-3.351	-3.351	0.001	(0)
H3SiO4-	2.467e-06	2.275e-06	-5.608	-5.643	-0.035	(0)
H2SiO4-2	5.435e-12	3.966e-12	-11.265	-11.402	-0.137	(0)
U(3)	0.000e+00					
U+3	0.000e+00	0.000e+00	-55.568	-55.885	-0.317	(0)
U(4)	1.458e-21					
U(OH)4	1.458e-21	1.460e-21	-20.836	-20.836	0.001	(0)
U(OH)3+	1.328e-25	1.224e-25	-24.877	-24.912	-0.035	(0)
U(OH)2+2	2.094e-30	1.514e-30	-29.679	-29.820	-0.141	(0)
U(CO3)4-4	2.986e-31	8.165e-32	-30.525	-31.088	-0.563	(0)
U(CO3)5-6	2.700e-35	1.460e-36	-34.569	-35.836	-1.267	(0)
UOH+3	4.927e-36	2.376e-36	-35.307	-35.624	-0.317	(0)
U(SO4)2	7.659e-40	7.670e-40	-39.116	-39.115	0.001	(0)
USO4+2	5.100e-40	3.688e-40	-39.292	-39.433	-0.141	(0)
U+4	0.000e+00	0.000e+00	-41.944	-42.507	-0.563	(0)
UCl+3	0.000e+00	0.000e+00	-43.668	-43.985	-0.317	(0)
U6(OH)15+9	0.000e+00	0.000e+00	-154.040	-156.891	-2.851	(0)
U(5)	9.900e-17					
UO2+	9.900e-17	9.130e-17	-16.004	-16.040	-0.035	(0)
UO2(CO3)3-5	1.202e-24	1.585e-25	-23.920	-24.800	-0.880	(0)
U(6)	9.834e-08					
UO2(CO3)3-4	4.916e-08	1.344e-08	-7.308	-7.872	-0.563	(0)
UO2(CO3)2-2	4.856e-08	3.512e-08	-7.314	-7.454	-0.141	(0)
UO2CO3	4.189e-10	4.195e-10	-9.378	-9.377	0.001	(0)
UO2(OH)3-	1.980e-10	1.826e-10	-9.703	-9.738	-0.035	(0)
UO2OH+	4.508e-12	4.157e-12	-11.346	-11.381	-0.035	(0)
UO2+2	3.408e-14	2.464e-14	-13.468	-13.608	-0.141	(0)
UO2SO4	9.284e-15	9.297e-15	-14.032	-14.032	0.001	(0)
UO2(OH)4-2	1.960e-16	1.417e-16	-15.708	-15.849	-0.141	(0)
UO2(SO4)2-2	3.545e-17	2.563e-17	-16.450	-16.591	-0.141	(0)
UO2Cl+	1.759e-17	1.622e-17	-16.755	-16.790	-0.035	(0)
(UO2)2(OH)2+2	2.754e-18	1.992e-18	-17.560	-17.701	-0.141	(0)
(UO2)3(CO3)6-6	1.659e-18	8.974e-20	-17.780	-19.047	-1.267	(0)
(UO2)3(OH)7-	1.096e-18	1.011e-18	-17.960	-17.995	-0.035	(0)
(UO2)3(OH)5+	3.249e-19	2.996e-19	-18.488	-18.523	-0.035	(0)
UO2Cl2	3.912e-22	3.918e-22	-21.408	-21.407	0.001	(0)
(UO2)3(OH)4+2	1.499e-22	1.084e-22	-21.824	-21.965	-0.141	(0)
(UO2)2OH+3	1.231e-22	5.934e-23	-21.910	-22.227	-0.317	(0)
(UO2)4(OH)7+	3.401e-23	3.137e-23	-22.468	-22.504	-0.035	(0)
Zn	6.320e-07					
Zn+2	3.114e-07	2.282e-07	-6.507	-6.642	-0.135	(0)
ZnCO3	1.938e-07	1.940e-07	-6.713	-6.712	0.001	(0)
ZnHCO3+	7.158e-08	6.601e-08	-7.145	-7.180	-0.035	(0)
Zn(CO3)2-2	2.445e-08	1.768e-08	-7.612	-7.752	-0.141	(0)
ZnSO4	1.714e-08	1.716e-08	-7.766	-7.765	0.001	(0)
Zn(OH)2	6.879e-09	6.888e-09	-8.162	-8.162	0.001	(0)
ZnOH+	6.362e-09	5.867e-09	-8.196	-8.232	-0.035	(0)
ZnCl+	2.144e-10	1.977e-10	-9.669	-9.704	-0.035	(0)
ZnOHCl	1.825e-10	1.827e-10	-9.739	-9.738	0.001	(0)
Zn(SO4)2-2	7.187e-11	5.197e-11	-10.143	-10.284	-0.141	(0)
Zn(OH)3-	1.157e-12	1.067e-12	-11.937	-11.972	-0.035	(0)

ZnCl2	9.818e-14	9.832e-14	-13.008	-13.007	0.001	(0)
ZnCl3-	5.575e-17	5.140e-17	-16.254	-16.289	-0.035	(0)
Zn(OH)4-2	1.145e-17	8.280e-18	-16.941	-17.082	-0.141	(0)
ZnCl4-2	1.619e-20	1.178e-20	-19.791	-19.929	-0.138	(0)

-------------------------------Saturation indices--------------------------------

Phase	SI**	log IAP	log K(288 K, 1 atm)	
Adularia	1.61	-19.70	-21.31	KAlSi3O8
Al(OH)3(a)	-1.04	10.39	11.43	Al(OH)3
AlAsO4:2H2O	-8.54	-24.37	-15.84	AlAsO4:2H2O
Albite	0.14	-18.48	-18.62	NaAlSi3O8
AlumK	-18.31	-23.66	-5.34	KAl(SO4)2:12H2O
Alunite	-2.68	-2.88	-0.20	KAl3(SO4)2(OH)6
Analcime	-2.00	-15.13	-13.14	NaAlSi2O6:H2O
Anglesite	-6.47	-14.31	-7.84	PbSO4
Anhydrite	-2.20	-6.54	-4.34	CaSO4
Annite	4.52	-82.62	-87.14	KFe3AlSi3O10(OH)2
Anorthite	-0.98	-20.97	-19.99	CaAl2Si2O8
Aragonite	-0.16	-8.45	-8.28	CaCO3
Arsenolite	-32.23	-33.78	-1.55	As2O3
Artinite	-8.03	2.25	10.29	MgCO3:Mg(OH)2:3H2O
As2O5(cr)	-35.55	-27.14	8.41	As2O5
As_native	-38.77	-51.96	-13.19	As
B-UO2(OH)2	-4.10	1.77	5.87	UO2(OH)2
Ba3(AsO4)2	7.34	-43.00	-50.34	Ba3(AsO4)2
Barite	0.13	-10.00	-10.13	BaSO4
Basaluminite	0.02	22.72	22.70	Al4(OH)10SO4
BaSeO3	-8.32	-14.71	-6.39	BaSeO3
Beidellite	5.02	-41.69	-46.71	(NaKMg0.5)0.11Al2.33Si3.67O10(OH)2
Bianchite	-8.34	-10.10	-1.76	ZnSO4:6H2O
Birnessite	-12.17	31.43	43.60	MnO2
Bixbyite	-12.52	-12.77	-0.25	Mn2O3
Boehmite	1.13	10.39	9.26	AlOOH
Brucite	-5.99	11.50	17.49	Mg(OH)2
Bunsenite	-6.78	6.24	13.02	NiO
Ca3(AsO4)2:4w	-13.71	-32.61	-18.91	Ca3(AsO4)2:4H2O
Calcite	-0.01	-8.45	-8.43	CaCO3
CaSeO3	-5.65	-11.25	-5.60	CaSeO3
Cd(gamma)	-30.70	-16.68	14.02	Cd
Cd(OH)2	-6.95	6.70	13.65	Cd(OH)2
Cd(OH)2(a)	-7.52	6.70	14.23	Cd(OH)2
Cd3(OH)2(SO4)2	-24.29	-17.58	6.71	Cd3(OH)2(SO4)2
Cd3(OH)4SO4	-21.30	1.26	22.56	Cd3(OH)4SO4
Cd4(OH)6SO4	-20.43	7.97	28.40	Cd4(OH)6SO4
CdCl2	-14.72	-15.29	-0.57	CdCl2
CdCl2:2.5H2O	-13.31	-15.29	-1.98	CdCl2:2.5H2O
CdCl2:H2O	-13.62	-15.29	-1.67	CdCl2:H2O
CdMetal	-30.60	-16.68	13.92	Cd
CdOHCl	-7.99	-4.29	3.70	CdOHCl
CdSiO3	-6.11	3.35	9.46	CdSiO3
CdSO4	-12.39	-12.14	0.25	CdSO4
CdSO4:2.7H2O	-10.37	-12.14	-1.77	CdSO4:2.67H2O
CdSO4:H2O	-10.66	-12.14	-1.48	CdSO4:H2O
Cerrusite	-2.97	-16.22	-13.25	PbCO3
Chalcedony	0.31	-3.35	-3.66	SiO2
Chlorite14A	-3.76	68.23	71.99	Mg5Al2Si3O10(OH)8
Chlorite7A	-7.22	68.23	75.46	Mg5Al2Si3O10(OH)8
Chrysotile	-5.60	27.80	33.40	Mg3Si2O5(OH)4
Claudetite	-32.28	-33.78	-1.50	As2O3
Clinoenstatite	-3.67	8.15	11.82	MgSiO3
CO2(g)	-2.57	-3.91	-1.35	CO2
Coffinite	-7.70	-15.10	-7.39	USiO4
Cotunnite	-12.56	-17.46	-4.90	PbCl2
Cristobalite	0.37	-3.35	-3.72	SiO2
Diaspore	2.92	10.39	7.47	AlOOH
Diopside	-3.56	17.10	20.67	CaMgSi2O6

Dolomite	-0.83	-17.70	-16.86	CaMg(CO3)2
Dolomite(d)	-1.42	-17.70	-16.28	CaMg(CO3)2
Epsomite	-5.13	-7.34	-2.21	MgSO4:7H2O
Fe(OH)2.7Cl.3	5.86	2.82	-3.04	Fe(OH)2.7Cl0.3
Fe(OH)3(a)	1.23	6.12	4.89	Fe(OH)3
Fe2(SeO3)3	-23.00	-58.43	-35.43	Fe2(SeO3)3
Fe3(OH)8	-0.31	19.91	20.22	Fe3(OH)8
FeSe2	-52.72	-71.30	-18.58	FeSe2
Forsterite	-9.81	19.65	29.47	Mg2SiO4
Gibbsite	1.74	10.39	8.65	Al(OH)3
Goethite	6.77	6.12	-0.65	FeOOH
Goslarite	-8.06	-10.10	-2.04	ZnSO4:7H2O
Greenalite	-4.48	16.33	20.81	Fe3Si2O5(OH)4
Gummite	-9.18	1.77	10.95	UO3
Gypsum	-1.95	-6.54	-4.58	CaSO4:2H2O
H2(g)	-23.38	-26.49	-3.11	H2
H2O(g)	-1.76	-0.00	1.76	H2O
Halite	-7.70	-6.14	1.56	NaCl
Halloysite	0.63	14.08	13.45	Al2Si2O5(OH)4
Hausmannite	-15.90	47.53	63.43	Mn3O4
Hematite	15.50	12.23	-3.27	Fe2O3
Huntite	-6.84	-36.19	-29.35	CaMg3(CO3)4
Hydrocerrusite	-10.45	-27.91	-17.46	Pb(OH)2:2PbCO3
Hydromagnesite	-17.98	-25.50	-7.52	Mg5(CO3)4(OH)2:4H2O
Illite	4.34	-37.23	-41.57	K0.6Mg0.25Al2.3Si3.5O10(OH)2
Jarosite(ss)	-6.56	-16.39	-9.83	(K0.77Na0.03H0.2)Fe3(SO4)2(OH)6
Jarosite-K	-7.23	-15.70	-8.46	KFe3(SO4)2(OH)6
Jarosite-Na	-10.06	-14.48	-4.42	NaFe3(SO4)2(OH)6
JarositeH	-15.26	-19.33	-4.07	(H3O)Fe3(SO4)2(OH)6
Jurbanite	-5.22	-8.45	-3.23	AlOHSO4
Kaolinite	5.80	14.08	8.28	Al2Si2O5(OH)4
Kmica	10.63	24.75	14.12	KAl3Si3O10(OH)2
Larnakite	-9.65	-9.78	-0.13	PbO:PbSO4
Laumontite	4.23	-27.67	-31.91	CaAl2Si4O12:4H2O
Laurionite	-7.09	-6.46	0.62	PbOHCl
Leonhardite	16.56	-55.35	-71.91	Ca2Al4Si8O24:7H2O
Litharge	-8.58	4.53	13.11	PbO
Magadiite	-4.30	-18.60	-14.30	NaSi7O13(OH)3:3H2O
Maghemite	5.85	12.23	6.39	Fe2O3
Magnesite	-1.37	-9.25	-7.88	MgCO3
Magnetite	14.97	19.91	4.94	Fe3O4
Manganite	-5.60	19.74	25.34	MnOOH
Massicot	-8.78	4.53	13.31	PbO
Melanterite	-8.83	-11.16	-2.33	FeSO4:7H2O
Minium	-39.17	36.97	76.14	Pb3O4
Mirabilite	-7.56	-9.13	-1.57	Na2SO4:10H2O
Mn2(SO4)3	-64.51	-69.29	-4.78	Mn2(SO4)3
Mn3(AsO4)2:8H2O	-16.66	-45.37	-28.71	Mn3(AsO4)2:8H2O
MnCl2:4H2O	-16.24	-13.94	2.30	MnCl2:4H2O
MnSO4	-13.83	-10.79	3.04	MnSO4
Monteponite	-7.66	6.70	14.36	CdO
Montmorillonite-Aberdeen	5.74	-23.95	-29.69	(HNaK)0.14Mg0.45Fe0.33Al1.47Si3.82O10(OH)2
Montmorillonite-BelleFourche	6.45	-28.46	-34.91	(HNaK)0.09Mg0.29Fe0.24Al1.57Si3.93O10(OH)2
Montmorillonite-Ca	5.19	-41.23	-46.42	Ca0.165Al2.33Si3.67O10(OH)2
Morenosite	-10.17	-12.61	-2.43	NiSO4:7H2O
Na4UO2(CO3)3	-24.77	-41.06	-16.29	Na4UO2(CO3)3
Nahcolite	-4.84	-5.47	-0.64	NaHCO3
Natron	-9.35	-11.04	-1.69	Na2CO3:10H2O
Nesquehonite	-3.77	-9.25	-5.48	MgCO3:3H2O
Ni(OH)2	-3.84	6.24	10.07	Ni(OH)2
Ni2SiO4	-6.21	9.12	15.34	Ni2SiO4
Ni3(AsO4)2:8H2O	-25.31	-50.82	-25.51	Ni3(AsO4)2:8H2O
Ni4(OH)6SO4	-25.90	6.10	32.00	Ni4(OH)6SO4
NiCO3	-7.91	-14.51	-6.60	NiCO3
Nsutite	-11.13	31.43	42.56	MnO2
O2(g)	-1.06	-3.88	-2.82	O2

Otavite	-1.95	-14.05	-12.10	CdCO3
Pb(OH)2	-3.95	4.53	8.48	Pb(OH)2
Pb2(OH)3Cl	-10.73	-1.93	8.79	Pb2(OH)3Cl
Pb2O(OH)2	-17.14	9.06	26.20	PbO:Pb(OH)2
Pb2O3	-28.60	32.44	61.04	Pb2O3
Pb2OCO3	-11.46	-11.69	-0.23	PbO:PbCO3
Pb2SiO4	-14.67	5.71	20.38	Pb2SiO4
Pb3(AsO4)2	-20.53	-55.93	-35.40	Pb3(AsO4)2
Pb3O2CO3	-18.81	-7.16	11.65	PbCO3:2PbO
Pb3O2SO4	-16.14	-5.25	10.90	PbSO4:2PbO
Pb4(OH)6SO4	-21.82	-0.72	21.10	Pb4(OH)6SO4
Pb4O3SO4	-23.65	-0.72	22.94	PbSO4:3PbO
PbMetal	-23.11	-18.85	4.26	Pb
PbO:0.3H2O	-8.45	4.53	12.98	PbO:0.33H2O
PbSiO3	-6.36	1.18	7.54	PbSiO3
Phillipsite	0.78	-19.09	-19.87	Na0.5K0.5AlSi3O8:H2O
Phlogopite	-5.83	38.48	44.31	KMg3AlSi3O10(OH)2
Phosgenite	-13.87	-33.68	-19.81	PbCl2:PbCO3
Plattnerite	-23.08	27.91	50.99	PbO2
Portlandite	-11.24	12.30	23.54	Ca(OH)2
Prehnite	-0.08	-12.02	-11.94	Ca2Al2Si3O10(OH)2
Pyrochroite	-7.15	8.05	15.20	Mn(OH)2
Pyrolusite	-11.50	31.43	42.93	MnO2
Pyrophyllite	8.34	-39.98	-48.31	Al2Si4O10(OH)2
Quartz	0.77	-3.35	-4.12	SiO2
Retgersite	-10.54	-12.61	-2.07	NiSO4:6H2O
Rhodochrosite	-1.60	-12.70	-11.10	MnCO3
Rhodochrosite(d)	-2.31	-12.70	-10.39	MnCO3
Rutherfordine	-4.56	-18.98	-14.42	UO2CO3
Schoepite	-3.92	1.77	5.69	UO2(OH)2:H2O
Scorodite	-8.40	-28.65	-20.25	FeAsO4:2H2O
Se(s)	-10.48	-27.80	-17.32	Se
SeO2	-15.18	-23.56	-8.38	SeO2
Sepiolite	-3.07	12.95	16.02	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-5.71	12.95	18.66	Mg2Si3O7.5OH:3H2O
Siderite	-2.24	-13.07	-10.83	FeCO3
Siderite(d)(3)	-2.62	-13.07	-10.45	FeCO3
Silicagel	-0.23	-3.35	-3.12	SiO2
SiO2(a)	-0.56	-3.35	-2.79	SiO2
Smithsonite	-2.12	-12.01	-9.90	ZnCO3
Talc	-1.40	21.10	22.51	Mg3Si4O10(OH)2
Thenardite	-8.96	-9.13	-0.17	Na2SO4
Thermonatrite	-11.23	-11.04	0.19	Na2CO3:H2O
Tremolite	-3.58	55.31	58.89	Ca2Mg5Si8O22(OH)2
Trona	-16.15	-16.51	-0.37	NaHCO3:Na2CO3:2H2O
U(OH)2SO4	-27.39	-30.59	-3.20	U(OH)2SO4
U3O8(c)	-11.78	11.52	23.30	U3O8
U4O9(c)	-22.64	-23.61	-0.97	U4O9
UO2(a)	-11.85	-11.75	0.10	UO2
UO3(gamma)	-6.41	1.77	8.18	UO3
Uraninite(c)	-7.39	-11.75	-4.36	UO2
Uranophane	-8.34	9.15	17.49	Ca(UO2)2(SiO3OH)2
Wairakite	-0.34	-27.67	-27.33	CaAl2Si4O12:2H2O
Willemite	-2.00	14.13	16.13	Zn2SiO4
Witherite	-3.31	-11.91	-8.59	BaCO3
Zincite(c)	-2.92	8.74	11.66	ZnO
Zincosite	-13.57	-10.10	3.47	ZnSO4
Zn(OH)2-a	-3.71	8.74	12.45	Zn(OH)2
Zn(OH)2-b	-3.01	8.74	11.75	Zn(OH)2
Zn(OH)2-c	-3.46	8.74	12.20	Zn(OH)2
Zn(OH)2-e	-2.76	8.74	11.50	Zn(OH)2
Zn(OH)2-g	-2.97	8.74	11.71	Zn(OH)2
Zn2(OH)2SO4	-8.86	-1.36	7.50	Zn2(OH)2SO4
Zn2(OH)3Cl	-8.72	6.48	15.20	Zn2(OH)3Cl
Zn3(AsO4)2:2.5w	-15.77	-43.31	-27.55	Zn3(AsO4)2:2.5H2O
Zn3O(SO4)2	-31.97	-11.47	20.50	ZnO:2ZnSO4
Zn4(OH)6SO4	-12.29	16.11	28.40	Zn4(OH)6SO4
Zn5(OH)8Cl2	-16.80	21.70	38.50	Zn5(OH)8Cl2

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  ZnCl2           -20.70    -13.25    7.45  ZnCl2
  ZnCO3:H2O        -1.75    -12.01  -10.26  ZnCO3:H2O
  ZnMetal         -41.28    -14.64   26.63  Zn
  ZnO(a)           -2.57      8.74   11.31  ZnO
  ZnSiO3            2.02      5.39    3.37  ZnSiO3
  ZnSO4:H2O        -9.79    -10.10   -0.32  ZnSO4:H2O

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
  For ideal gases, phi = 1.

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End of simulation.
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Reading input data for simulation 2.
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End of Run after 0.094 Seconds.
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```

```
   Input file: E:\Project Stuff\Models\Trace Metal_Inputst.pqi
  Output file: E:\Project Stuff\Models\Trace Metal_Inputst.pqo
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.1.2-8538\database
\wateq4f.dat

------------------
Reading data base.
------------------

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

      DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 3.1.2-8538\database
\wateq4f.dat
      TITLE Professional Project Geochemical Model
      SOLUTION   MW-4
              units   ppm
              pH      7.69
              temp    15.6
              O(0)            7.13
              Ca              41.6
              Mg              3.9
              Na              28.4
              K               3.76
              Ba              0.0253
              Cd              0
              Cu              0
              Zn              0.00853
              Pb              0.000191
              Mn              0.00436
              Se              0.00195
              Ni              0.000703
              Fe              0
              Al              0.00712
              U               0.00974
              As              0.00272
              Cl              13.8
              Alkalinity      132.4 as HCO3
              S(6)            32.3
              Si              26.1
      END
-----
TITLE
-----

 Professional Project Geochemical Model

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Beginning of initial solution calculations.
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Initial solution 1.     MW-4

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

      Elements           Molality       Moles

      Al                2.640e-07   2.640e-07
```

Alkalinity	2.170e-03	2.170e-03
As	3.632e-08	3.632e-08
Ba	1.843e-07	1.843e-07
Ca	1.038e-03	1.038e-03
Cl	3.894e-04	3.894e-04
K	9.619e-05	9.619e-05
Mg	1.605e-04	1.605e-04
Mn	7.939e-08	7.939e-08
Na	1.236e-03	1.236e-03
Ni	1.198e-08	1.198e-08
O(0)	4.458e-04	4.458e-04
Pb	9.221e-10	9.221e-10
S(6)	3.363e-04	3.363e-04
Se	2.470e-08	2.470e-08
Si	4.345e-04	4.345e-04
U	4.093e-08	4.093e-08
Zn	1.305e-07	1.305e-07

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

pH	= 7.690
pe	= 4.000
Activity of water	= 1.000
Ionic strength	= 4.825e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 2.262e-03
Total CO2 (mol/kg)	= 2.262e-03
Temperature (°C)	= 15.60
Electrical balance (eq)	= 4.984e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 7.37
Iterations	= 14
Total H	= 1.110163e+02
Total O	= 5.551643e+01

----------Redox couples----------

Redox couple	pe	Eh (volts)
O(-2)/O(0)	13.7212	0.7861

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	2.501e-07	2.321e-07	-6.602	-6.634	-0.032	(0)
H+	2.183e-08	2.042e-08	-7.661	-7.690	-0.029	0.00
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.03
Al	2.640e-07					
Al(OH)4-	2.602e-07	2.419e-07	-6.585	-6.616	-0.032	(0)
Al(OH)3	2.898e-09	2.901e-09	-8.538	-8.537	0.000	(0)
Al(OH)2+	9.031e-10	8.407e-10	-9.044	-9.075	-0.031	(0)
AlOH+2	6.949e-12	5.220e-12	-11.158	-11.282	-0.124	(0)
Al+3	3.650e-14	2.003e-14	-13.438	-13.698	-0.261	(0)
AlSO4+	1.349e-14	1.254e-14	-13.870	-13.902	-0.032	(0)
Al(SO4)2-	9.161e-17	8.517e-17	-16.038	-16.070	-0.032	(0)
AlHSO4+2	2.837e-23	2.115e-23	-22.547	-22.675	-0.128	(0)
As(3)	1.223e-17					
H3AsO3	1.192e-17	1.193e-17	-16.924	-16.923	0.000	(0)
H2AsO3-	3.101e-19	2.882e-19	-18.508	-18.540	-0.032	(0)
H4AsO3+	1.299e-25	1.207e-25	-24.886	-24.918	-0.032	(0)
HAsO3-2	2.486e-26	1.853e-26	-25.605	-25.732	-0.128	(0)
AsO3-3	2.515e-34	1.299e-34	-33.600	-33.887	-0.287	(0)
As(5)	3.632e-08					
HAsO4-2	2.912e-08	2.171e-08	-7.536	-7.663	-0.128	(0)
H2AsO4-	7.192e-09	6.683e-09	-8.143	-8.175	-0.032	(0)
AsO4-3	3.629e-12	1.874e-12	-11.440	-11.727	-0.287	(0)
H3AsO4	2.479e-14	2.481e-14	-13.606	-13.605	0.000	(0)

Ba	1.843e-07					
Ba+2	1.680e-07	1.259e-07	-6.775	-6.900	-0.125	(0)
BaSO4	1.416e-08	1.417e-08	-7.849	-7.849	0.000	(0)
BaHCO3+	1.913e-09	1.778e-09	-8.718	-8.750	-0.032	(0)
BaCO3	1.976e-10	1.978e-10	-9.704	-9.704	0.000	(0)
BaOH+	2.245e-13	2.089e-13	-12.649	-12.680	-0.031	(0)
C(4)	2.262e-03					
HCO3-	2.127e-03	1.980e-03	-2.672	-2.703	-0.031	(0)
CO2	1.048e-04	1.049e-04	-3.980	-3.979	0.000	(0)
CaHCO3+	1.685e-05	1.570e-05	-4.773	-4.804	-0.031	(0)
CO3-2	4.889e-06	3.673e-06	-5.311	-5.435	-0.124	(0)
CaCO3	3.905e-06	3.910e-06	-5.408	-5.408	0.000	(0)
MgHCO3+	2.776e-06	2.579e-06	-5.557	-5.589	-0.032	(0)
NaHCO3	1.275e-06	1.277e-06	-5.894	-5.894	0.000	(0)
MgCO3	3.483e-07	3.487e-07	-6.458	-6.458	0.000	(0)
NaCO3-	5.162e-08	4.805e-08	-7.287	-7.318	-0.031	(0)
ZnCO3	3.803e-08	3.807e-08	-7.420	-7.419	0.000	(0)
UO2(CO3)2-2	2.259e-08	1.684e-08	-7.646	-7.774	-0.128	(0)
UO2(CO3)3-4	1.798e-08	5.554e-09	-7.745	-8.255	-0.510	(0)
ZnHCO3+	1.394e-08	1.295e-08	-7.856	-7.888	-0.032	(0)
MnCO3	1.255e-08	1.256e-08	-7.901	-7.901	0.000	(0)
NiCO3	1.119e-08	1.120e-08	-7.951	-7.951	0.000	(0)
MnHCO3+	8.170e-09	7.601e-09	-8.088	-8.119	-0.031	(0)
Zn(CO3)2-2	4.010e-09	2.989e-09	-8.397	-8.524	-0.128	(0)
BaHCO3+	1.913e-09	1.778e-09	-8.718	-8.750	-0.032	(0)
PbCO3	8.550e-10	8.559e-10	-9.068	-9.068	0.000	(0)
UO2CO3	2.332e-10	2.334e-10	-9.632	-9.632	0.000	(0)
BaCO3	1.976e-10	1.978e-10	-9.704	-9.704	0.000	(0)
NiHCO3+	1.210e-10	1.125e-10	-9.917	-9.949	-0.032	(0)
Ni(CO3)2-2	9.591e-11	7.150e-11	-10.018	-10.146	-0.128	(0)
PbHCO3+	2.270e-11	2.109e-11	-10.644	-10.676	-0.032	(0)
Pb(CO3)2-2	1.059e-11	7.896e-12	-10.975	-11.103	-0.128	(0)
(UO2)3(CO3)6-6	1.391e-19	9.892e-21	-18.857	-20.005	-1.148	(0)
UO2(CO3)3-5	4.104e-25	6.547e-26	-24.387	-25.184	-0.797	(0)
U(CO3)4-4	9.410e-32	2.906e-32	-31.026	-31.537	-0.510	(0)
U(CO3)5-6	6.297e-36	4.478e-37	-35.201	-36.349	-1.148	(0)
Ca	1.038e-03					
Ca+2	9.872e-04	7.411e-04	-3.006	-3.130	-0.124	(0)
CaSO4	3.030e-05	3.034e-05	-4.519	-4.518	0.000	(0)
CaHCO3+	1.685e-05	1.570e-05	-4.773	-4.804	-0.031	(0)
CaCO3	3.905e-06	3.910e-06	-5.408	-5.408	0.000	(0)
CaOH+	6.465e-09	6.023e-09	-8.189	-8.220	-0.031	(0)
CaHSO4+	3.511e-12	3.263e-12	-11.455	-11.486	-0.032	(0)
Cl	3.894e-04					
Cl-	3.894e-04	3.615e-04	-3.410	-3.442	-0.032	(0)
MnCl+	6.817e-11	6.343e-11	-10.166	-10.198	-0.031	(0)
ZnCl+	3.547e-11	3.295e-11	-10.450	-10.482	-0.032	(0)
ZnOHCl	3.042e-11	3.046e-11	-10.517	-10.516	0.000	(0)
NiCl+	4.021e-13	3.736e-13	-12.396	-12.428	-0.032	(0)
PbCl+	1.633e-13	1.517e-13	-12.787	-12.819	-0.032	(0)
ZnCl2	1.198e-14	1.200e-14	-13.921	-13.921	0.000	(0)
MnCl2	9.998e-15	1.001e-14	-14.000	-14.000	0.000	(0)
NiCl2	4.899e-16	4.904e-16	-15.310	-15.309	0.000	(0)
PbCl2	1.041e-16	1.042e-16	-15.983	-15.982	0.000	(0)
UO2Cl+	8.251e-18	7.666e-18	-17.084	-17.115	-0.032	(0)
ZnCl3-	4.941e-18	4.590e-18	-17.306	-17.338	-0.032	(0)
MnCl3-	1.071e-18	9.966e-19	-17.970	-18.001	-0.031	(0)
PbCl3-	3.033e-20	2.818e-20	-19.518	-19.550	-0.032	(0)
ZnCl4-2	1.028e-21	7.701e-22	-20.988	-21.113	-0.125	(0)
UO2Cl2	1.354e-22	1.356e-22	-21.868	-21.868	0.000	(0)
PbCl4-2	6.071e-24	4.526e-24	-23.217	-23.344	-0.128	(0)
UCl+3	0.000e+00	0.000e+00	-44.023	-44.310	-0.287	(0)
H(0)	6.494e-27					
H2	3.247e-27	3.251e-27	-26.489	-26.488	0.000	(0)
K	9.619e-05					
K+	9.606e-05	8.919e-05	-4.017	-4.050	-0.032	(0)
KSO4-	1.276e-07	1.188e-07	-6.894	-6.925	-0.031	(0)
Mg	1.605e-04					

Mg+2	1.526e-04	1.150e-04	-3.816	-3.939	-0.123	(0)
MgSO4	4.709e-06	4.714e-06	-5.327	-5.327	0.000	(0)
MgHCO3+	2.776e-06	2.579e-06	-5.557	-5.589	-0.032	(0)
MgCO3	3.483e-07	3.487e-07	-6.458	-6.458	0.000	(0)
MgOH+	9.125e-09	8.509e-09	-8.040	-8.070	-0.030	(0)
Mn(2)	7.939e-08					
Mn+2	5.714e-08	4.307e-08	-7.243	-7.366	-0.123	(0)
MnCO3	1.255e-08	1.256e-08	-7.901	-7.901	0.000	(0)
MnHCO3+	8.170e-09	7.601e-09	-8.088	-8.119	-0.031	(0)
MnSO4	1.428e-09	1.430e-09	-8.845	-8.845	0.000	(0)
MnCl+	6.817e-11	6.343e-11	-10.166	-10.198	-0.031	(0)
MnOH+	2.641e-11	2.458e-11	-10.578	-10.609	-0.031	(0)
MnCl2	9.998e-15	1.001e-14	-14.000	-14.000	0.000	(0)
MnCl3-	1.071e-18	9.966e-19	-17.970	-18.001	-0.031	(0)
Mn(OH)3-	8.617e-20	8.017e-20	-19.065	-19.096	-0.031	(0)
Mn(3)	5.877e-30					
Mn+3	5.877e-30	3.225e-30	-29.231	-29.491	-0.261	(0)
Mn(6)	0.000e+00					
MnO4-2	0.000e+00	0.000e+00	-51.740	-51.866	-0.125	(0)
Mn(7)	0.000e+00					
MnO4-	0.000e+00	0.000e+00	-57.852	-57.884	-0.033	(0)
Na	1.236e-03					
Na+	1.233e-03	1.146e-03	-2.909	-2.941	-0.032	(0)
NaSO4-	1.304e-06	1.214e-06	-5.885	-5.916	-0.031	(0)
NaHCO3	1.275e-06	1.277e-06	-5.894	-5.894	0.000	(0)
NaCO3-	5.162e-08	4.805e-08	-7.287	-7.318	-0.031	(0)
Ni	1.198e-08					
NiCO3	1.119e-08	1.120e-08	-7.951	-7.951	0.000	(0)
Ni+2	5.520e-10	4.115e-10	-9.258	-9.386	-0.128	(0)
NiHCO3+	1.210e-10	1.125e-10	-9.917	-9.949	-0.032	(0)
Ni(CO3)2-2	9.591e-11	7.150e-11	-10.018	-10.146	-0.128	(0)
NiSO4	1.656e-11	1.658e-11	-10.781	-10.780	0.000	(0)
NiOH+	1.513e-12	1.406e-12	-11.820	-11.852	-0.032	(0)
NiCl+	4.021e-13	3.736e-13	-12.396	-12.428	-0.032	(0)
Ni(OH)2	9.858e-14	9.869e-14	-13.006	-13.006	0.000	(0)
NiCl2	4.899e-16	4.904e-16	-15.310	-15.309	0.000	(0)
Ni(SO4)2-2	2.916e-16	2.174e-16	-15.535	-15.663	-0.128	(0)
Ni(OH)3-	5.201e-17	4.833e-17	-16.284	-16.316	-0.032	(0)
O(0)	4.458e-04					
O2	2.229e-04	2.231e-04	-3.652	-3.651	0.000	(0)
Pb	9.221e-10					
PbCO3	8.550e-10	8.559e-10	-9.068	-9.068	0.000	(0)
PbHCO3+	2.270e-11	2.109e-11	-10.644	-10.676	-0.032	(0)
Pb+2	1.799e-11	1.341e-11	-10.745	-10.873	-0.128	(0)
PbOH+	1.378e-11	1.281e-11	-10.861	-10.893	-0.032	(0)
Pb(CO3)2-2	1.059e-11	7.896e-12	-10.975	-11.103	-0.128	(0)
PbSO4	1.692e-12	1.694e-12	-11.772	-11.771	0.000	(0)
Pb(OH)2	2.437e-13	2.440e-13	-12.613	-12.613	0.000	(0)
PbCl+	1.633e-13	1.517e-13	-12.787	-12.819	-0.032	(0)
Pb(SO4)2-2	2.679e-15	1.997e-15	-14.572	-14.700	-0.128	(0)
Pb(OH)3-	1.476e-16	1.372e-16	-15.831	-15.863	-0.032	(0)
PbCl2	1.041e-16	1.042e-16	-15.983	-15.982	0.000	(0)
PbCl3-	3.033e-20	2.818e-20	-19.518	-19.550	-0.032	(0)
Pb(OH)4-2	2.065e-20	1.539e-20	-19.685	-19.813	-0.128	(0)
Pb2OH+3	7.445e-21	3.845e-21	-20.128	-20.415	-0.287	(0)
PbCl4-2	6.071e-24	4.526e-24	-23.217	-23.344	-0.128	(0)
Pb3(OH)4+2	5.720e-27	4.264e-27	-26.243	-26.370	-0.128	(0)
S(6)	3.363e-04					
SO4-2	2.999e-04	2.246e-04	-3.523	-3.649	-0.125	(0)
CaSO4	3.030e-05	3.034e-05	-4.519	-4.518	0.000	(0)
MgSO4	4.709e-06	4.714e-06	-5.327	-5.327	0.000	(0)
NaSO4-	1.304e-06	1.214e-06	-5.885	-5.916	-0.031	(0)
KSO4-	1.276e-07	1.188e-07	-6.894	-6.925	-0.031	(0)
BaSO4	1.416e-08	1.417e-08	-7.849	-7.849	0.000	(0)
ZnSO4	2.536e-09	2.539e-09	-8.596	-8.595	0.000	(0)
MnSO4	1.428e-09	1.430e-09	-8.845	-8.845	0.000	(0)
HSO4-	3.939e-10	3.662e-10	-9.405	-9.436	-0.032	(0)
NiSO4	1.656e-11	1.658e-11	-10.781	-10.780	0.000	(0)

Zn(SO4)2-2	6.700e-12	4.995e-12	-11.174	-11.301	-0.128	(0)
CaHSO4+	3.511e-12	3.263e-12	-11.455	-11.486	-0.032	(0)
PbSO4	1.692e-12	1.694e-12	-11.772	-11.771	0.000	(0)
AlSO4+	1.349e-14	1.254e-14	-13.870	-13.902	-0.032	(0)
UO2SO4	3.896e-15	3.901e-15	-14.409	-14.409	0.000	(0)
Pb(SO4)2-2	2.679e-15	1.997e-15	-14.572	-14.700	-0.128	(0)
Ni(SO4)2-2	2.916e-16	2.174e-16	-15.535	-15.663	-0.128	(0)
Al(SO4)2-	9.161e-17	8.517e-17	-16.038	-16.070	-0.032	(0)
UO2(SO4)2-2	9.372e-18	6.987e-18	-17.028	-17.156	-0.128	(0)
AlHSO4+2	2.837e-23	2.115e-23	-22.547	-22.675	-0.128	(0)
U(SO4)2	2.088e-40	2.091e-40	-39.680	-39.680	0.000	(0)
USO4+2	2.076e-40	1.547e-40	-39.683	-39.810	-0.128	(0)
Se(-2)	0.000e+00					
HSe-	0.000e+00	0.000e+00	-43.810	-43.842	-0.032	(0)
H2Se	0.000e+00	0.000e+00	-47.606	-47.605	0.000	(0)
Se(4)	2.470e-08					
HSeO3-	2.071e-08	1.924e-08	-7.684	-7.716	-0.032	(0)
SeO3-2	3.997e-09	2.980e-09	-8.398	-8.526	-0.128	(0)
H2SeO3	2.207e-13	2.209e-13	-12.656	-12.656	0.000	(0)
Se(6)	5.318e-16					
SeO4-2	5.318e-16	3.964e-16	-15.274	-15.402	-0.128	(0)
HSeO4-	3.040e-22	2.825e-22	-21.517	-21.549	-0.032	(0)
Si	4.345e-04					
H4SiO4	4.321e-04	4.326e-04	-3.364	-3.364	0.000	(0)
H3SiO4-	2.375e-06	2.206e-06	-5.624	-5.656	-0.032	(0)
H2SiO4-2	5.122e-12	3.847e-12	-11.291	-11.415	-0.124	(0)
U(3)	0.000e+00					
U+3	0.000e+00	0.000e+00	-55.788	-56.075	-0.287	(0)
U(4)	9.420e-22					
U(OH)4	9.419e-22	9.429e-22	-21.026	-21.026	0.000	(0)
U(OH)3+	8.509e-26	7.907e-26	-25.070	-25.102	-0.032	(0)
U(OH)2+2	1.312e-30	9.779e-31	-29.882	-30.010	-0.128	(0)
U(CO3)4-4	9.410e-32	2.906e-32	-31.026	-31.537	-0.510	(0)
U(CO3)5-6	6.297e-36	4.478e-37	-35.201	-36.349	-1.148	(0)
UOH+3	2.971e-36	1.534e-36	-35.527	-35.814	-0.287	(0)
U(SO4)2	2.088e-40	2.091e-40	-39.680	-39.680	0.000	(0)
USO4+2	2.076e-40	1.547e-40	-39.683	-39.810	-0.128	(0)
U+4	0.000e+00	0.000e+00	-42.186	-42.697	-0.510	(0)
UCl+3	0.000e+00	0.000e+00	-44.023	-44.310	-0.287	(0)
U6(OH)15+9	0.000e+00	0.000e+00	-155.447	-158.030	-2.583	(0)
U(5)	6.345e-17					
UO2+	6.345e-17	5.896e-17	-16.198	-16.229	-0.032	(0)
UO2(CO3)3-5	4.104e-25	6.547e-26	-24.387	-25.184	-0.797	(0)
U(6)	4.093e-08					
UO2(CO3)2-2	2.259e-08	1.684e-08	-7.646	-7.774	-0.128	(0)
UO2(CO3)3-4	1.798e-08	5.554e-09	-7.745	-8.255	-0.510	(0)
UO2CO3	2.332e-10	2.334e-10	-9.632	-9.632	0.000	(0)
UO2(OH)3-	1.269e-10	1.179e-10	-9.896	-9.928	-0.032	(0)
UO2OH+	2.890e-12	2.685e-12	-11.539	-11.571	-0.032	(0)
UO2+2	2.135e-14	1.592e-14	-13.671	-13.798	-0.128	(0)
UO2SO4	3.896e-15	3.901e-15	-14.409	-14.409	0.000	(0)
UO2(OH)4-2	1.228e-16	9.155e-17	-15.911	-16.038	-0.128	(0)
UO2(SO4)2-2	9.372e-18	6.987e-18	-17.028	-17.156	-0.128	(0)
UO2Cl+	8.251e-18	7.666e-18	-17.084	-17.115	-0.032	(0)
(UO2)2(OH)2+2	1.114e-18	8.307e-19	-17.953	-18.081	-0.128	(0)
(UO2)3(OH)7-	2.931e-19	2.724e-19	-18.533	-18.565	-0.032	(0)
(UO2)3(CO3)6-6	1.391e-19	9.892e-21	-18.857	-20.005	-1.148	(0)
(UO2)3(OH)5+	8.686e-20	8.071e-20	-19.061	-19.093	-0.032	(0)
UO2Cl2	1.354e-22	1.356e-22	-21.868	-21.868	0.000	(0)
(UO2)2OH+3	4.793e-23	2.475e-23	-22.319	-22.606	-0.287	(0)
(UO2)3(OH)4+2	3.916e-23	2.919e-23	-22.407	-22.535	-0.128	(0)
(UO2)4(OH)7+	5.873e-24	5.457e-24	-23.231	-23.263	-0.032	(0)
Zn	1.305e-07					
Zn+2	6.893e-08	5.196e-08	-7.162	-7.284	-0.123	(0)
ZnCO3	3.803e-08	3.807e-08	-7.420	-7.419	0.000	(0)
ZnHCO3+	1.394e-08	1.295e-08	-7.856	-7.888	-0.032	(0)
Zn(CO3)2-2	4.010e-09	2.989e-09	-8.397	-8.524	-0.128	(0)
ZnSO4	2.536e-09	2.539e-09	-8.596	-8.595	0.000	(0)

Zn(OH)2	1.567e-09	1.569e-09	-8.805	-8.804	0.000	(0)
ZnOH+	1.438e-09	1.336e-09	-8.842	-8.874	-0.032	(0)
ZnCl+	3.547e-11	3.295e-11	-10.450	-10.482	-0.032	(0)
ZnOHCl	3.042e-11	3.046e-11	-10.517	-10.516	0.000	(0)
Zn(SO4)2-2	6.700e-12	4.995e-12	-11.174	-11.301	-0.128	(0)
Zn(OH)3-	2.614e-13	2.429e-13	-12.583	-12.615	-0.032	(0)
ZnCl2	1.198e-14	1.200e-14	-13.921	-13.921	0.000	(0)
ZnCl3-	4.941e-18	4.590e-18	-17.306	-17.338	-0.032	(0)
Zn(OH)4-2	2.529e-18	1.886e-18	-17.597	-17.725	-0.128	(0)
ZnCl4-2	1.028e-21	7.701e-22	-20.988	-21.113	-0.125	(0)

Saturation indices

Phase	SI**	log IAP	log K(288 K, 1 atm)	
Adularia	0.55	-20.76	-21.31	KAlSi3O8
Al(OH)3(a)	-2.06	9.37	11.43	Al(OH)3
AlAsO4:2H2O	-9.59	-25.43	-15.84	AlAsO4:2H2O
Albite	-1.03	-19.65	-18.62	NaAlSi3O8
AlumK	-19.70	-25.05	-5.34	KAl(SO4)2:12H2O
Alunite	-6.10	-6.30	-0.20	KAl3(SO4)2(OH)6
Analcime	-3.15	-16.28	-13.14	NaAlSi2O6:H2O
Anglesite	-6.68	-14.52	-7.84	PbSO4
Anhydrite	-2.44	-6.78	-4.34	CaSO4
Anorthite	-3.10	-23.09	-19.99	CaAl2Si2O8
Aragonite	-0.28	-8.57	-8.28	CaCO3
Arsenolite	-32.30	-33.85	-1.55	As2O3
Artinite	-8.22	2.07	10.29	MgCO3:Mg(OH)2:3H2O
As2O5(cr)	-35.62	-27.21	8.41	As2O5
As_native	-38.80	-51.99	-13.19	As
B-UO2(OH)2	-4.29	1.58	5.87	UO2(OH)2
Ba3(AsO4)2	6.18	-44.15	-50.34	Ba3(AsO4)2
Barite	-0.42	-10.55	-10.13	BaSO4
Basaluminite	-4.24	18.46	22.70	Al4(OH)10SO4
BaSeO3	-9.04	-15.43	-6.39	BaSeO3
Beidellite	2.59	-44.13	-46.71	(NaKMg0.5)0.11Al2.33Si3.67O10(OH)2
Bianchite	-9.17	-10.93	-1.76	ZnSO4:6H2O
Birnessite	-12.21	31.39	43.60	MnO2
Bixbyite	-12.60	-12.84	-0.25	Mn2O3
Boehmite	0.12	9.37	9.26	AlOOH
Brucite	-6.05	11.44	17.49	Mg(OH)2
Bunsenite	-7.03	5.99	13.02	NiO
Ca3(AsO4)2:4w	-13.94	-32.84	-18.91	Ca3(AsO4)2:4H2O
Calcite	-0.13	-8.57	-8.43	CaCO3
CaSeO3	-6.06	-11.66	-5.60	CaSeO3
Cerrusite	-3.06	-16.31	-13.25	PbCO3
Chalcedony	0.30	-3.36	-3.66	SiO2
Chlorite14A	-6.14	65.85	71.99	Mg5Al2Si3O10(OH)8
Chlorite7A	-9.60	65.85	75.46	Mg5Al2Si3O10(OH)8
Chrysotile	-5.81	27.59	33.40	Mg3Si2O5(OH)4
Claudetite	-32.34	-33.85	-1.50	As2O3
Clinoenstatite	-3.74	8.08	11.82	MgSiO3
CO2(g)	-2.63	-3.98	-1.35	CO2
Coffinite	-7.91	-15.30	-7.39	USiO4
Cotunnite	-12.85	-17.76	-4.90	PbCl2
Cristobalite	0.35	-3.36	-3.72	SiO2
Diaspore	1.90	9.37	7.47	AlOOH
Diopside	-3.70	16.96	20.67	CaMgSi2O6
Dolomite	-1.07	-17.94	-16.86	CaMg(CO3)2
Dolomite(d)	-1.66	-17.94	-16.28	CaMg(CO3)2
Epsomite	-5.38	-7.59	-2.21	MgSO4:7H2O
Forsterite	-9.95	19.52	29.47	Mg2SiO4
Gibbsite	0.72	9.37	8.65	Al(OH)3
Goslarite	-8.89	-10.93	-2.04	ZnSO4:7H2O
Gummite	-9.37	1.58	10.95	UO3
Gypsum	-2.19	-6.78	-4.58	CaSO4:2H2O
H2(g)	-23.38	-26.49	-3.11	H2
H2O(g)	-1.76	-0.00	1.76	H2O

Halite	-7.94	-6.38	1.56	NaCl
Halloysite	-1.44	12.02	13.45	Al2Si2O5(OH)4
Hausmannite	-16.01	47.42	63.43	Mn3O4
Huntite	-7.34	-36.69	-29.35	CaMg3(CO3)4
Hydrocerrusite	-10.65	-28.11	-17.46	Pb(OH)2:2PbCO3
Hydromagnesite	-18.54	-26.06	-7.52	Mg5(CO3)4(OH)2:4H2O
Illite	1.94	-39.63	-41.57	K0.6Mg0.25Al2.3Si3.5O10(OH)2
Jurbanite	-6.43	-9.66	-3.23	AlOHSO4
Kaolinite	3.74	12.02	8.28	Al2Si2O5(OH)4
Kmica	7.54	21.66	14.12	KAl3Si3O10(OH)2
Larnakite	-9.89	-10.01	-0.13	PbO:PbSO4
Laumontite	2.09	-29.82	-31.91	CaAl2Si4O12:4H2O
Laurionite	-7.25	-6.62	0.62	PbOHCl
Leonhardite	12.27	-59.64	-71.91	Ca2Al4Si8O24:7H2O
Litharge	-8.60	4.51	13.11	PbO
Magadiite	-4.50	-18.80	-14.30	NaSi7O13(OH)3:3H2O
Magnesite	-1.49	-9.37	-7.88	MgCO3
Manganite	-5.64	19.70	25.34	MnOOH
Massicot	-8.80	4.51	13.31	PbO
Minium	-39.24	36.90	76.14	Pb3O4
Mirabilite	-7.96	-9.53	-1.57	Na2SO4:10H2O
Mn2(SO4)3	-65.15	-69.93	-4.78	Mn2(SO4)3
Mn3(AsO4)2:8H2O	-16.85	-45.55	-28.71	Mn3(AsO4)2:8H2O
MnCl2:4H2O	-16.55	-14.25	2.30	MnCl2:4H2O
MnSO4	-14.05	-11.01	3.04	MnSO4
Montmorillonite-Ca	2.76	-43.66	-46.42	Ca0.165Al2.33Si3.67O10(OH)2
Morenosite	-10.60	-13.03	-2.43	NiSO4:7H2O
Na4UO2(CO3)3	-25.58	-41.87	-16.29	Na4UO2(CO3)3
Nahcolite	-5.01	-5.64	-0.64	NaHCO3
Natron	-9.63	-11.32	-1.69	Na2CO3:10H2O
Nesquehonite	-3.89	-9.37	-5.48	MgCO3:3H2O
Ni(OH)2	-4.08	5.99	10.07	Ni(OH)2
Ni2SiO4	-6.71	8.62	15.34	Ni2SiO4
Ni3(AsO4)2:8H2O	-26.10	-51.61	-25.51	Ni3(AsO4)2:8H2O
Ni4(OH)6SO4	-27.05	4.95	32.00	Ni4(OH)6SO4
NiCO3	-8.22	-14.82	-6.60	NiCO3
Nsutite	-11.17	31.39	42.56	MnO2
O2(g)	-0.83	-3.65	-2.82	O2
Pb(OH)2	-3.98	4.51	8.48	Pb(OH)2
Pb2(OH)3Cl	-10.91	-2.12	8.79	Pb2(OH)3Cl
Pb2O(OH)2	-17.19	9.01	26.20	PbO:Pb(OH)2
Pb2O3	-28.65	32.39	61.04	Pb2O3
Pb2OCO3	-11.57	-11.80	-0.23	PbO:PbCO3
Pb2SiO4	-14.73	5.65	20.38	Pb2SiO4
Pb3(AsO4)2	-20.67	-56.07	-35.40	Pb3(AsO4)2
Pb3O2CO3	-18.94	-7.29	11.65	PbCO3:2PbO
Pb3O2SO4	-16.40	-5.51	10.90	PbSO4:2PbO
Pb4(OH)6SO4	-22.10	-1.00	21.10	Pb4(OH)6SO4
Pb4O3SO4	-23.94	-1.00	22.94	PbSO4:3PbO
PbMetal	-23.13	-18.87	4.26	Pb
PbO:0.3H2O	-8.47	4.51	12.98	PbO:0.33H2O
PbSiO3	-6.40	1.14	7.54	PbSiO3
Phillipsite	-0.33	-20.20	-19.87	Na0.5K0.5AlSi3O8:H2O
Phlogopite	-7.07	37.24	44.31	KMg3AlSi3O10(OH)2
Phosgenite	-14.25	-34.06	-19.81	PbCl2:PbCO3
Plattnerite	-23.10	27.89	50.99	PbO2
Portlandite	-11.29	12.25	23.54	Ca(OH)2
Prehnite	-2.26	-14.20	-11.94	Ca2Al2Si3O10(OH)2
Pyrochroite	-7.19	8.01	15.20	Mn(OH)2
Pyrolusite	-11.54	31.39	42.93	MnO2
Pyrophyllite	6.25	-42.07	-48.31	Al2Si4O10(OH)2
Quartz	0.76	-3.36	-4.12	SiO2
Retgersite	-10.97	-13.03	-2.07	NiSO4:6H2O
Rhodochrosite	-1.70	-12.80	-11.10	MnCO3
Rhodochrosite(d)	-2.41	-12.80	-10.39	MnCO3
Rutherfordine	-4.82	-19.23	-14.42	UO2CO3
Schoepite	-4.11	1.58	5.69	UO2(OH)2:H2O
Se(s)	-10.83	-28.15	-17.32	Se

SeO2	-15.53	-23.91	-8.38	SeO2
Sepiolite	-3.23	12.79	16.02	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-5.87	12.79	18.66	Mg2Si3O7.5OH:3H2O
Silicagel	-0.24	-3.36	-3.12	SiO2
SiO2(a)	-0.57	-3.36	-2.79	SiO2
Smithsonite	-2.82	-12.72	-9.90	ZnCO3
Talc	-1.64	20.87	22.51	Mg3Si4O10(OH)2
Thenardite	-9.36	-9.53	-0.17	Na2SO4
Thermonatrite	-11.51	-11.32	0.19	Na2CO3:H2O
Tremolite	-4.09	54.79	58.89	Ca2Mg5Si8O22(OH)2
Trona	-16.59	-16.96	-0.37	NaHCO3:Na2CO3:2H2O
U(OH)2SO4	-27.77	-30.97	-3.20	U(OH)2SO4
U3O8(c)	-12.35	10.95	23.30	U3O8
U4O9(c)	-23.40	-24.37	-0.97	U4O9
UO2(a)	-12.04	-11.94	0.10	UO2
UO3(gamma)	-6.60	1.58	8.18	UO3
Uraninite(c)	-7.58	-11.94	-4.36	UO2
Uranophane	-8.80	8.69	17.49	Ca(UO2)2(SiO3OH)2
Wairakite	-2.49	-29.82	-27.33	CaAl2Si4O12:2H2O
Willemite	-3.30	12.83	16.13	Zn2SiO4
Witherite	-3.74	-12.34	-8.59	BaCO3
Zincite(c)	-3.57	8.10	11.66	ZnO
Zincosite	-14.40	-10.93	3.47	ZnSO4
Zn(OH)2-a	-4.35	8.10	12.45	Zn(OH)2
Zn(OH)2-b	-3.65	8.10	11.75	Zn(OH)2
Zn(OH)2-c	-4.10	8.10	12.20	Zn(OH)2
Zn(OH)2-e	-3.40	8.10	11.50	Zn(OH)2
Zn(OH)2-g	-3.61	8.10	11.71	Zn(OH)2
Zn2(OH)2SO4	-10.34	-2.84	7.50	Zn2(OH)2SO4
Zn2(OH)3Cl	-10.14	5.06	15.20	Zn2(OH)3Cl
Zn3(AsO4)2:2.5w	-17.76	-45.31	-27.55	Zn3(AsO4)2:2.5H2O
Zn3O(SO4)2	-34.27	-13.77	20.50	ZnO:2ZnSO4
Zn4(OH)6SO4	-15.05	13.35	28.40	Zn4(OH)6SO4
Zn5(OH)8Cl2	-20.29	18.21	38.50	Zn5(OH)8Cl2
ZnCl2	-21.62	-14.17	7.45	ZnCl2
ZnCO3:H2O	-2.46	-12.72	-10.26	ZnCO3:H2O
ZnMetal	-41.92	-15.28	26.63	Zn
ZnO(a)	-3.21	8.10	11.31	ZnO
ZnSiO3	1.37	4.73	3.37	ZnSiO3
ZnSO4:H2O	-10.62	-10.93	-0.32	ZnSO4:H2O

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
  For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.111 Seconds.

```
   Input file: E:\Project Stuff\Models\Trace Metal_Inputst.pqi
  Output file: E:\Project Stuff\Models\Trace Metal_Inputst.pqo
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.1.2-8538\database
\wateq4f.dat

------------------
Reading data base.
------------------

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

      DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 3.1.2-8538\database
\wateq4f.dat
      TITLE Professional Project Geochemical Model
      SOLUTION   Windmill Well
              units   ppm
              pH      7.65
              temp    13.4
              O(0)            6.6
              Ca              60.4
              Mg              5.57
              Na              39
              K               2.93
              Ba              0.0856
              Cd              0.00012
              Cu              0.00148
              Zn              0.135
              Pb              0.000157
              Mn              0.041
              Se              0.00409
              Ni              0.00132
              Fe              0.026
              Al              0
              U               0.0177
              As              0.00145
              Cl              15.3
              Alkalinity      143.3 as HCO3
              S(6)            66.5
              Si              22.4
      END
-----
TITLE
-----

 Professional Project Geochemical Model

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

Initial solution 1.     Windmill Well

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

      Elements           Molality       Moles

      Alkalinity        2.349e-03   2.349e-03
```

As	1.936e-08	1.936e-08
Ba	6.235e-07	6.235e-07
Ca	1.508e-03	1.508e-03
Cd	1.068e-09	1.068e-09
Cl	4.317e-04	4.317e-04
Cu	2.330e-08	2.330e-08
Fe	4.657e-07	4.657e-07
K	7.496e-05	7.496e-05
Mg	2.292e-04	2.292e-04
Mn	7.466e-07	7.466e-07
Na	1.697e-03	1.697e-03
Ni	2.249e-08	2.249e-08
O(0)	4.126e-04	4.126e-04
Pb	7.580e-10	7.580e-10
S(6)	6.925e-04	6.925e-04
Se	5.182e-08	5.182e-08
Si	3.729e-04	3.729e-04
U	7.439e-08	7.439e-08
Zn	2.066e-06	2.066e-06

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

pH	= 7.650
pe	= 4.000
Activity of water	= 1.000
Ionic strength	= 6.710e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 2.464e-03
Total CO2 (mol/kg)	= 2.464e-03
Temperature (°C)	= 13.40
Electrical balance (eq)	= 1.087e-03
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 12.11
Iterations	= 13
Total H	= 1.110162e+02
Total O	= 5.551816e+01

----------Redox couples----------

Redox couple	pe	Eh (volts)
O(-2)/O(0)	13.9487	0.7930

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	1.916e-07	1.758e-07	-6.718	-6.755	-0.037	(0)
H+	2.416e-08	2.239e-08	-7.617	-7.650	-0.033	0.00
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.03
As(3)	1.301e-17					
H3AsO3	1.273e-17	1.275e-17	-16.895	-16.894	0.001	(0)
H2AsO3-	2.800e-19	2.572e-19	-18.553	-18.590	-0.037	(0)
H4AsO3+	1.540e-25	1.415e-25	-24.813	-24.849	-0.037	(0)
HAsO3-2	1.913e-26	1.362e-26	-25.718	-25.866	-0.148	(0)
AsO3-3	1.724e-34	8.030e-35	-33.763	-34.095	-0.332	(0)
As(5)	1.936e-08					
HAsO4-2	1.531e-08	1.090e-08	-7.815	-7.963	-0.148	(0)
H2AsO4-	4.048e-09	3.718e-09	-8.393	-8.430	-0.037	(0)
AsO4-3	1.739e-12	8.099e-13	-11.760	-12.092	-0.332	(0)
H3AsO4	1.478e-14	1.480e-14	-13.830	-13.830	0.001	(0)
Ba	6.235e-07					
Ba+2	5.346e-07	3.832e-07	-6.272	-6.417	-0.145	(0)
BaSO4	8.246e-08	8.259e-08	-7.084	-7.083	0.001	(0)
BaHCO3+	5.867e-09	5.390e-09	-8.232	-8.268	-0.037	(0)
BaCO3	5.286e-10	5.294e-10	-9.277	-9.276	0.001	(0)
BaOH+	6.303e-13	5.799e-13	-12.200	-12.237	-0.036	(0)
C(4)	2.464e-03					

HCO3-	2.296e-03	2.114e-03	-2.639	-2.675	-0.036	(0)
CO2	1.278e-04	1.280e-04	-3.893	-3.893	0.001	(0)
CaHCO3+	2.347e-05	2.164e-05	-4.629	-4.665	-0.035	(0)
CaCO3	4.760e-06	4.768e-06	-5.322	-5.322	0.001	(0)
CO3-2	4.695e-06	3.376e-06	-5.328	-5.472	-0.143	(0)
MgHCO3+	3.998e-06	3.671e-06	-5.398	-5.435	-0.037	(0)
NaHCO3	1.846e-06	1.849e-06	-5.734	-5.733	0.001	(0)
ZnCO3	5.438e-07	5.446e-07	-6.265	-6.264	0.001	(0)
MgCO3	4.146e-07	4.152e-07	-6.382	-6.382	0.001	(0)
ZnHCO3+	2.343e-07	2.152e-07	-6.630	-6.667	-0.037	(0)
MnCO3	1.041e-07	1.043e-07	-6.982	-6.982	0.001	(0)
MnHCO3+	7.962e-08	7.326e-08	-7.099	-7.135	-0.036	(0)
NaCO3-	5.776e-08	5.319e-08	-7.238	-7.274	-0.036	(0)
Zn(CO3)2-2	5.521e-08	3.931e-08	-7.258	-7.406	-0.148	(0)
UO2(CO3)3-4	3.702e-08	9.513e-09	-7.432	-8.022	-0.590	(0)
UO2(CO3)2-2	3.676e-08	2.617e-08	-7.435	-7.582	-0.148	(0)
FeHCO3+	2.255e-08	2.072e-08	-7.647	-7.684	-0.037	(0)
NiCO3	2.082e-08	2.085e-08	-7.682	-7.681	0.001	(0)
FeCO3	7.924e-09	7.936e-09	-8.101	-8.100	0.001	(0)
CuCO3	6.696e-09	6.706e-09	-8.174	-8.174	0.001	(0)
BaHCO3+	5.867e-09	5.390e-09	-8.232	-8.268	-0.037	(0)
PbCO3	6.968e-10	6.979e-10	-9.157	-9.156	0.001	(0)
BaCO3	5.286e-10	5.294e-10	-9.277	-9.276	0.001	(0)
CuHCO3+	4.267e-10	3.919e-10	-9.370	-9.407	-0.037	(0)
UO2CO3	4.115e-10	4.121e-10	-9.386	-9.385	0.001	(0)
NiHCO3+	2.647e-10	2.431e-10	-9.577	-9.614	-0.037	(0)
Ni(CO3)2-2	1.718e-10	1.223e-10	-9.765	-9.913	-0.148	(0)
CdHCO3+	4.746e-11	4.359e-11	-10.324	-10.361	-0.037	(0)
Cu(CO3)2-2	4.003e-11	2.850e-11	-10.398	-10.545	-0.148	(0)
PbHCO3+	2.175e-11	1.997e-11	-10.663	-10.700	-0.037	(0)
Pb(CO3)2-2	8.311e-12	5.917e-12	-11.080	-11.228	-0.148	(0)
CdCO3	1.746e-12	1.749e-12	-11.758	-11.757	0.001	(0)
Cd(CO3)2-2	2.622e-14	1.867e-14	-13.581	-13.729	-0.148	(0)
(UO2)3(CO3)6-6	9.437e-19	4.437e-20	-18.025	-19.353	-1.328	(0)
UO2(CO3)3-5	8.290e-25	9.920e-26	-24.081	-25.003	-0.922	(0)
U(CO3)4-4	3.611e-31	9.279e-32	-30.442	-31.033	-0.590	(0)
U(CO3)5-6	2.139e-35	1.006e-36	-34.670	-35.998	-1.328	(0)
Ca	1.508e-03					
Ca+2	1.402e-03	1.008e-03	-2.853	-2.997	-0.144	(0)
CaSO4	7.711e-05	7.723e-05	-4.113	-4.112	0.001	(0)
CaHCO3+	2.347e-05	2.164e-05	-4.629	-4.665	-0.035	(0)
CaCO3	4.760e-06	4.768e-06	-5.322	-5.322	0.001	(0)
CaOH+	8.101e-09	7.468e-09	-8.091	-8.127	-0.035	(0)
CaHSO4+	9.704e-12	8.914e-12	-11.013	-11.050	-0.037	(0)
Cd	1.068e-09					
Cd+2	9.160e-10	6.522e-10	-9.038	-9.186	-0.148	(0)
CdSO4	7.501e-11	7.512e-11	-10.125	-10.124	0.001	(0)
CdHCO3+	4.746e-11	4.359e-11	-10.324	-10.361	-0.037	(0)
CdCl+	2.580e-11	2.369e-11	-10.588	-10.625	-0.037	(0)
CdCO3	1.746e-12	1.749e-12	-11.758	-11.757	0.001	(0)
CdOH+	1.078e-12	9.899e-13	-11.968	-12.004	-0.037	(0)
Cd(SO4)2-2	5.356e-13	3.813e-13	-12.271	-12.419	-0.148	(0)
CdOHCl	3.375e-13	3.380e-13	-12.472	-12.471	0.001	(0)
CdCl2	3.737e-14	3.743e-14	-13.427	-13.427	0.001	(0)
Cd(CO3)2-2	2.622e-14	1.867e-14	-13.581	-13.729	-0.148	(0)
Cd(OH)2	5.802e-15	5.811e-15	-14.236	-14.236	0.001	(0)
CdCl3-	8.491e-18	7.799e-18	-17.071	-17.108	-0.037	(0)
Cd(OH)3-	3.170e-20	2.912e-20	-19.499	-19.536	-0.037	(0)
Cd2OH+3	7.892e-21	3.675e-21	-20.103	-20.435	-0.332	(0)
Cd(OH)4-2	1.628e-26	1.159e-26	-25.788	-25.936	-0.148	(0)
Cl	4.317e-04					
Cl-	4.317e-04	3.961e-04	-3.365	-3.402	-0.037	(0)
MnCl+	6.820e-10	6.275e-10	-9.166	-9.202	-0.036	(0)
ZnCl+	5.514e-10	5.063e-10	-9.259	-9.296	-0.037	(0)
ZnOHCl	4.730e-10	4.737e-10	-9.325	-9.325	0.001	(0)
FeCl+	5.824e-11	5.358e-11	-10.235	-10.271	-0.036	(0)
CdCl+	2.580e-11	2.369e-11	-10.588	-10.625	-0.037	(0)
CuCl2-	9.645e-13	8.856e-13	-12.016	-12.053	-0.037	(0)

NiCl+	9.025e-13	8.290e-13	-12.045	-12.081	-0.037	(0)
CdOHCl	3.375e-13	3.380e-13	-12.472	-12.471	0.001	(0)
CuCl+	2.378e-13	2.184e-13	-12.624	-12.661	-0.037	(0)
ZnCl2	1.997e-13	2.001e-13	-12.700	-12.699	0.001	(0)
PbCl+	1.514e-13	1.391e-13	-12.820	-12.857	-0.037	(0)
MnCl2	1.083e-13	1.085e-13	-12.965	-12.965	0.001	(0)
CdCl2	3.737e-14	3.743e-14	-13.427	-13.427	0.001	(0)
NiCl2	1.190e-15	1.192e-15	-14.924	-14.924	0.001	(0)
CuCl3-2	7.405e-16	5.307e-16	-15.130	-15.275	-0.145	(0)
PbCl2	1.092e-16	1.094e-16	-15.962	-15.961	0.001	(0)
ZnCl3-	9.006e-17	8.270e-17	-16.045	-16.082	-0.037	(0)
CuCl2	4.071e-17	4.078e-17	-16.390	-16.390	0.001	(0)
UO2Cl+	1.740e-17	1.598e-17	-16.759	-16.796	-0.037	(0)
MnCl3-	1.286e-17	1.184e-17	-16.891	-16.927	-0.036	(0)
CdCl3-	8.491e-18	7.799e-18	-17.071	-17.108	-0.037	(0)
FeCl+2	5.499e-19	3.941e-19	-18.260	-18.404	-0.145	(0)
PbCl3-	3.478e-20	3.195e-20	-19.459	-19.496	-0.037	(0)
ZnCl4-2	2.082e-20	1.492e-20	-19.682	-19.826	-0.145	(0)
FeCl2+	1.113e-21	1.022e-21	-20.954	-20.990	-0.037	(0)
UO2Cl2	3.023e-22	3.027e-22	-21.520	-21.519	0.001	(0)
CuCl3-	5.039e-23	4.627e-23	-22.298	-22.335	-0.037	(0)
PbCl4-2	7.752e-24	5.519e-24	-23.111	-23.258	-0.148	(0)
FeCl3	4.043e-26	4.050e-26	-25.393	-25.393	0.001	(0)
CuCl4-2	9.692e-29	6.947e-29	-28.014	-28.158	-0.145	(0)
UCl+3	0.000e+00	0.000e+00	-43.262	-43.593	-0.332	(0)
Cu(1)	1.991e-11					
Cu+	1.895e-11	1.734e-11	-10.722	-10.761	-0.038	(0)
CuCl2-	9.645e-13	8.856e-13	-12.016	-12.053	-0.037	(0)
CuCl3-2	7.405e-16	5.307e-16	-15.130	-15.275	-0.145	(0)
Cu(2)	2.328e-08					
Cu(OH)2	1.539e-08	1.542e-08	-7.813	-7.812	0.001	(0)
CuCO3	6.696e-09	6.706e-09	-8.174	-8.174	0.001	(0)
Cu+2	5.122e-10	3.699e-10	-9.291	-9.432	-0.141	(0)
CuHCO3+	4.267e-10	3.919e-10	-9.370	-9.407	-0.037	(0)
CuOH+	1.799e-10	1.652e-10	-9.745	-9.782	-0.037	(0)
Cu(CO3)2-2	4.003e-11	2.850e-11	-10.398	-10.545	-0.148	(0)
CuSO4	2.984e-11	2.988e-11	-10.525	-10.525	0.001	(0)
CuCl+	2.378e-13	2.184e-13	-12.624	-12.661	-0.037	(0)
Cu(OH)3-	4.517e-14	4.149e-14	-13.345	-13.382	-0.037	(0)
Cu2(OH)2+2	5.062e-15	3.604e-15	-14.296	-14.443	-0.148	(0)
CuCl2	4.071e-17	4.078e-17	-16.390	-16.390	0.001	(0)
Cu(OH)4-2	5.193e-19	3.697e-19	-18.285	-18.432	-0.148	(0)
CuCl3-	5.039e-23	4.627e-23	-22.298	-22.335	-0.037	(0)
CuCl4-2	9.692e-29	6.947e-29	-28.014	-28.158	-0.145	(0)
Fe(2)	1.728e-07					
Fe+2	1.357e-07	9.800e-08	-6.867	-7.009	-0.141	(0)
FeHCO3+	2.255e-08	2.072e-08	-7.647	-7.684	-0.037	(0)
FeCO3	7.924e-09	7.936e-09	-8.101	-8.100	0.001	(0)
FeSO4	6.000e-09	6.010e-09	-8.222	-8.221	0.001	(0)
FeOH+	6.104e-10	5.617e-10	-9.214	-9.251	-0.036	(0)
FeCl+	5.824e-11	5.358e-11	-10.235	-10.271	-0.036	(0)
Fe(OH)2	7.462e-14	7.473e-14	-13.127	-13.126	0.001	(0)
FeHSO4+	9.439e-16	8.670e-16	-15.025	-15.062	-0.037	(0)
Fe(OH)3-	1.197e-16	1.101e-16	-15.922	-15.958	-0.036	(0)
Fe(3)	2.929e-07					
Fe(OH)3	2.174e-07	2.177e-07	-6.663	-6.662	0.001	(0)
Fe(OH)2+	6.955e-08	6.405e-08	-7.158	-7.194	-0.036	(0)
Fe(OH)4-	5.930e-09	5.460e-09	-8.227	-8.263	-0.036	(0)
FeOH+2	9.549e-12	6.845e-12	-11.020	-11.165	-0.145	(0)
FeSO4+	1.895e-16	1.744e-16	-15.722	-15.759	-0.036	(0)
Fe+3	9.579e-17	4.831e-17	-16.019	-16.316	-0.297	(0)
Fe(SO4)2-	1.703e-18	1.565e-18	-17.769	-17.806	-0.037	(0)
FeCl+2	5.499e-19	3.941e-19	-18.260	-18.404	-0.145	(0)
Fe2(OH)2+4	8.080e-21	2.076e-21	-20.093	-20.683	-0.590	(0)
FeCl2+	1.113e-21	1.022e-21	-20.954	-20.990	-0.037	(0)
FeHSO4+2	1.508e-23	1.073e-23	-22.822	-22.969	-0.148	(0)
Fe3(OH)4+5	7.072e-25	8.461e-26	-24.150	-25.073	-0.922	(0)
FeCl3	4.043e-26	4.050e-26	-25.393	-25.393	0.001	(0)

H(0)	7.990e-27					
H2	3.995e-27	4.001e-27	-26.398	-26.398	0.001	(0)
K	7.496e-05					
K+	7.478e-05	6.861e-05	-4.126	-4.164	-0.037	(0)
KSO4-	1.824e-07	1.679e-07	-6.739	-6.775	-0.036	(0)
Mg	2.292e-04					
Mg+2	2.134e-04	1.540e-04	-3.671	-3.812	-0.142	(0)
MgSO4	1.136e-05	1.138e-05	-4.945	-4.944	0.001	(0)
MgHCO3+	3.998e-06	3.671e-06	-5.398	-5.435	-0.037	(0)
MgCO3	4.146e-07	4.152e-07	-6.382	-6.382	0.001	(0)
MgOH+	9.102e-09	8.399e-09	-8.041	-8.076	-0.035	(0)
Mn(2)	7.466e-07					
Mn+2	5.384e-07	3.889e-07	-6.269	-6.410	-0.141	(0)
MnCO3	1.041e-07	1.043e-07	-6.982	-6.982	0.001	(0)
MnHCO3+	7.962e-08	7.326e-08	-7.099	-7.135	-0.036	(0)
MnSO4	2.358e-08	2.362e-08	-7.627	-7.627	0.001	(0)
MnCl+	6.820e-10	6.275e-10	-9.166	-9.202	-0.036	(0)
MnOH+	1.814e-10	1.669e-10	-9.741	-9.778	-0.036	(0)
MnCl2	1.083e-13	1.085e-13	-12.965	-12.965	0.001	(0)
MnCl3-	1.286e-17	1.184e-17	-16.891	-16.927	-0.036	(0)
Mn(OH)3-	5.967e-19	5.491e-19	-18.224	-18.260	-0.036	(0)
Mn(3)	4.089e-29					
Mn+3	4.089e-29	2.062e-29	-28.388	-28.686	-0.297	(0)
Mn(6)	0.000e+00					
MnO4-2	0.000e+00	0.000e+00	-51.957	-52.102	-0.145	(0)
Mn(7)	0.000e+00					
MnO4-	0.000e+00	0.000e+00	-58.237	-58.275	-0.038	(0)
Na	1.697e-03					
Na+	1.692e-03	1.555e-03	-2.772	-2.808	-0.037	(0)
NaSO4-	3.372e-06	3.105e-06	-5.472	-5.508	-0.036	(0)
NaHCO3	1.846e-06	1.849e-06	-5.734	-5.733	0.001	(0)
NaCO3-	5.776e-08	5.319e-08	-7.238	-7.274	-0.036	(0)
Ni	2.249e-08					
NiCO3	2.082e-08	2.085e-08	-7.682	-7.681	0.001	(0)
Ni+2	1.170e-09	8.332e-10	-8.932	-9.079	-0.148	(0)
NiHCO3+	2.647e-10	2.431e-10	-9.577	-9.614	-0.037	(0)
Ni(CO3)2-2	1.718e-10	1.223e-10	-9.765	-9.913	-0.148	(0)
NiSO4	6.287e-11	6.297e-11	-10.202	-10.201	0.001	(0)
NiOH+	2.394e-12	2.199e-12	-11.621	-11.658	-0.037	(0)
NiCl+	9.025e-13	8.290e-13	-12.045	-12.081	-0.037	(0)
Ni(OH)2	1.659e-13	1.662e-13	-12.780	-12.779	0.001	(0)
Ni(SO4)2-2	2.266e-15	1.613e-15	-14.645	-14.792	-0.148	(0)
NiCl2	1.190e-15	1.192e-15	-14.924	-14.924	0.001	(0)
Ni(OH)3-	8.081e-17	7.423e-17	-16.093	-16.129	-0.037	(0)
O(0)	4.126e-04					
O2	2.063e-04	2.066e-04	-3.685	-3.685	0.001	(0)
Pb	7.580e-10					
PbCO3	6.968e-10	6.979e-10	-9.157	-9.156	0.001	(0)
PbHCO3+	2.175e-11	1.997e-11	-10.663	-10.700	-0.037	(0)
Pb+2	1.671e-11	1.190e-11	-10.777	-10.925	-0.148	(0)
PbOH+	1.128e-11	1.036e-11	-10.948	-10.985	-0.037	(0)
Pb(CO3)2-2	8.311e-12	5.917e-12	-11.080	-11.228	-0.148	(0)
PbSO4	2.872e-12	2.877e-12	-11.542	-11.541	0.001	(0)
Pb(OH)2	1.797e-13	1.800e-13	-12.745	-12.745	0.001	(0)
PbCl+	1.514e-13	1.391e-13	-12.820	-12.857	-0.037	(0)
Pb(SO4)2-2	9.117e-15	6.491e-15	-14.040	-14.188	-0.148	(0)
PbCl2	1.092e-16	1.094e-16	-15.962	-15.961	0.001	(0)
Pb(OH)3-	1.005e-16	9.231e-17	-15.998	-16.035	-0.037	(0)
PbCl3-	3.478e-20	3.195e-20	-19.459	-19.496	-0.037	(0)
Pb(OH)4-2	1.326e-20	9.444e-21	-19.877	-20.025	-0.148	(0)
Pb2OH+3	5.925e-21	2.759e-21	-20.227	-20.559	-0.332	(0)
PbCl4-2	7.752e-24	5.519e-24	-23.111	-23.258	-0.148	(0)
Pb3(OH)4+2	2.029e-27	1.444e-27	-26.693	-26.840	-0.148	(0)
S(6)	6.925e-04					
SO4-2	6.003e-04	4.300e-04	-3.222	-3.367	-0.145	(0)
CaSO4	7.711e-05	7.723e-05	-4.113	-4.112	0.001	(0)
MgSO4	1.136e-05	1.138e-05	-4.945	-4.944	0.001	(0)
NaSO4-	3.372e-06	3.105e-06	-5.472	-5.508	-0.036	(0)

KSO4-	1.824e-07	1.679e-07	-6.739	-6.775	-0.036	(0)
BaSO4	8.246e-08	8.259e-08	-7.084	-7.083	0.001	(0)
ZnSO4	7.416e-08	7.428e-08	-7.130	-7.129	0.001	(0)
MnSO4	2.358e-08	2.362e-08	-7.627	-7.627	0.001	(0)
FeSO4	6.000e-09	6.010e-09	-8.222	-8.221	0.001	(0)
HSO4-	8.005e-10	7.359e-10	-9.097	-9.133	-0.037	(0)
Zn(SO4)2-2	4.001e-10	2.849e-10	-9.398	-9.545	-0.148	(0)
CdSO4	7.501e-11	7.512e-11	-10.125	-10.124	0.001	(0)
NiSO4	6.287e-11	6.297e-11	-10.202	-10.201	0.001	(0)
CuSO4	2.984e-11	2.988e-11	-10.525	-10.525	0.001	(0)
CaHSO4+	9.704e-12	8.914e-12	-11.013	-11.050	-0.037	(0)
PbSO4	2.872e-12	2.877e-12	-11.542	-11.541	0.001	(0)
Cd(SO4)2-2	5.356e-13	3.813e-13	-12.271	-12.419	-0.148	(0)
UO2SO4	1.367e-14	1.369e-14	-13.864	-13.864	0.001	(0)
Pb(SO4)2-2	9.117e-15	6.491e-15	-14.040	-14.188	-0.148	(0)
Ni(SO4)2-2	2.266e-15	1.613e-15	-14.645	-14.792	-0.148	(0)
FeHSO4+	9.439e-16	8.670e-16	-15.025	-15.062	-0.037	(0)
FeSO4+	1.895e-16	1.744e-16	-15.722	-15.759	-0.036	(0)
UO2(SO4)2-2	6.273e-17	4.467e-17	-16.202	-16.350	-0.148	(0)
Fe(SO4)2-	1.703e-18	1.565e-18	-17.769	-17.806	-0.037	(0)
FeHSO4+2	1.508e-23	1.073e-23	-22.822	-22.969	-0.148	(0)
U(SO4)2	3.082e-39	3.087e-39	-38.511	-38.510	0.001	(0)
USO4+2	1.814e-39	1.292e-39	-38.741	-38.889	-0.148	(0)
Se(-2)	0.000e+00					
HSe-	0.000e+00	0.000e+00	-43.244	-43.281	-0.037	(0)
H2Se	0.000e+00	0.000e+00	-46.974	-46.974	0.001	(0)
Se(4)	5.182e-08					
HSeO3-	4.383e-08	4.026e-08	-7.358	-7.395	-0.037	(0)
SeO3-2	7.988e-09	5.687e-09	-8.098	-8.245	-0.148	(0)
H2SeO3	5.061e-13	5.069e-13	-12.296	-12.295	0.001	(0)
Se(6)	8.838e-16					
SeO4-2	8.838e-16	6.293e-16	-15.054	-15.201	-0.148	(0)
HSeO4-	5.012e-22	4.604e-22	-21.300	-21.337	-0.037	(0)
Si	3.729e-04					
H4SiO4	3.712e-04	3.718e-04	-3.430	-3.430	0.001	(0)
H3SiO4-	1.725e-06	1.584e-06	-5.763	-5.800	-0.037	(0)
H2SiO4-2	2.978e-12	2.142e-12	-11.526	-11.669	-0.143	(0)
U(3)	0.000e+00					
U+3	0.000e+00	0.000e+00	-55.234	-55.566	-0.332	(0)
U(4)	2.092e-21					
U(OH)4	2.091e-21	2.095e-21	-20.680	-20.679	0.001	(0)
U(OH)3+	2.157e-25	1.981e-25	-24.666	-24.703	-0.037	(0)
U(OH)2+2	4.030e-30	2.870e-30	-29.395	-29.542	-0.148	(0)
U(CO3)4-4	3.611e-31	9.279e-32	-30.442	-31.033	-0.590	(0)
U(CO3)5-6	2.139e-35	1.006e-36	-34.670	-35.998	-1.328	(0)
UOH+3	1.157e-35	5.387e-36	-34.937	-35.269	-0.332	(0)
U(SO4)2	3.082e-39	3.087e-39	-38.511	-38.510	0.001	(0)
USO4+2	1.814e-39	1.292e-39	-38.741	-38.889	-0.148	(0)
U+4	0.000e+00	0.000e+00	-41.456	-42.046	-0.590	(0)
UCl+3	0.000e+00	0.000e+00	-43.262	-43.593	-0.332	(0)
U6(OH)15+9	0.000e+00	0.000e+00	-151.739	-154.727	-2.988	(0)
U(5)	1.309e-16					
UO2+	1.309e-16	1.203e-16	-15.883	-15.920	-0.037	(0)
UO2(CO3)3-5	8.290e-25	9.920e-26	-24.081	-25.003	-0.922	(0)
U(6)	7.439e-08					
UO2(CO3)3-4	3.702e-08	9.513e-09	-7.432	-8.022	-0.590	(0)
UO2(CO3)2-2	3.676e-08	2.617e-08	-7.435	-7.582	-0.148	(0)
UO2CO3	4.115e-10	4.121e-10	-9.386	-9.385	0.001	(0)
UO2(OH)3-	1.901e-10	1.746e-10	-9.721	-9.758	-0.037	(0)
UO2OH+	4.490e-12	4.125e-12	-11.348	-11.385	-0.037	(0)
UO2+2	4.363e-14	3.107e-14	-13.360	-13.508	-0.148	(0)
UO2SO4	1.367e-14	1.369e-14	-13.864	-13.864	0.001	(0)
UO2(OH)4-2	1.736e-16	1.236e-16	-15.760	-15.908	-0.148	(0)
UO2(SO4)2-2	6.273e-17	4.467e-17	-16.202	-16.350	-0.148	(0)
UO2Cl+	1.740e-17	1.598e-17	-16.759	-16.796	-0.037	(0)
(UO2)2(OH)2+2	3.224e-18	2.296e-18	-17.492	-17.639	-0.148	(0)
(UO2)3(OH)7-	1.157e-18	1.063e-18	-17.937	-17.974	-0.037	(0)
(UO2)3(CO3)6-6	9.437e-19	4.437e-20	-18.025	-19.353	-1.328	(0)

(UO2)3(OH)5+	2.947e-19	2.707e-19	-18.531	-18.567	-0.037 (0)
UO2Cl2	3.023e-22	3.027e-22	-21.520	-21.519	0.001 (0)
(UO2)3(OH)4+2	2.109e-22	1.502e-22	-21.676	-21.823	-0.148 (0)
(UO2)2OH+3	1.847e-22	8.600e-23	-21.734	-22.065	-0.332 (0)
(UO2)4(OH)7+	4.525e-23	4.156e-23	-22.344	-22.381	-0.037 (0)
Zn 2.066e-06					
Zn+2	1.120e-06	8.086e-07	-5.951	-6.092	-0.141 (0)
ZnCO3	5.438e-07	5.446e-07	-6.265	-6.264	0.001 (0)
ZnHCO3+	2.343e-07	2.152e-07	-6.630	-6.667	-0.037 (0)
ZnSO4	7.416e-08	7.428e-08	-7.130	-7.129	0.001 (0)
Zn(CO3)2-2	5.521e-08	3.931e-08	-7.258	-7.406	-0.148 (0)
Zn(OH)2	2.027e-08	2.031e-08	-7.693	-7.692	0.001 (0)
ZnOH+	1.726e-08	1.585e-08	-7.763	-7.800	-0.037 (0)
ZnCl+	5.514e-10	5.063e-10	-9.259	-9.296	-0.037 (0)
ZnOHCl	4.730e-10	4.737e-10	-9.325	-9.325	0.001 (0)
Zn(SO4)2-2	4.001e-10	2.849e-10	-9.398	-9.545	-0.148 (0)
Zn(OH)3-	3.122e-12	2.868e-12	-11.506	-11.542	-0.037 (0)
ZnCl2	1.997e-13	2.001e-13	-12.700	-12.699	0.001 (0)
ZnCl3-	9.006e-17	8.270e-17	-16.045	-16.082	-0.037 (0)
Zn(OH)4-2	2.851e-17	2.030e-17	-16.545	-16.692	-0.148 (0)
ZnCl4-2	2.082e-20	1.492e-20	-19.682	-19.826	-0.145 (0)

----------Saturation indices----------

Phase	SI**	log IAP	log K(286 K, 1 atm)	
Anglesite	-6.44	-14.29	-7.85	PbSO4
Anhydrite	-2.03	-6.36	-4.33	CaSO4
Antlerite	-9.35	-1.06	8.29	Cu3(OH)4SO4
Aragonite	-0.20	-8.47	-8.27	CaCO3
Arsenolite	-32.20	-33.79	-1.59	As2O3
Artinite	-8.25	2.20	10.45	MgCO3:Mg(OH)2:3H2O
As2O5(cr)	-36.11	-27.66	8.45	As2O5
As_native	-38.50	-51.84	-13.35	As
Atacamite	-7.21	0.68	7.89	Cu2(OH)3Cl
Azurite	-7.71	-3.05	4.67	Cu3(OH)2(CO3)2
B-UO2(OH)2	-4.16	1.79	5.95	UO2(OH)2
Ba3(AsO4)2	6.96	-43.43	-50.39	Ba3(AsO4)2
Barite	0.39	-9.78	-10.18	BaSO4
BaSeO3	-8.27	-14.66	-6.39	BaSeO3
Bianchite	-7.70	-9.46	-1.76	ZnSO4:6H2O
Birnessite	-11.41	32.19	43.60	MnO2
Bixbyite	-11.31	-11.47	-0.16	Mn2O3
Brochantite	-10.53	4.81	15.34	Cu4(OH)6SO4
Brucite	-6.16	11.49	17.64	Mg(OH)2
Bunsenite	-6.94	6.22	13.16	NiO
Ca3(AsO4)2:4w	-14.27	-33.17	-18.91	Ca3(AsO4)2:4H2O
Calcite	-0.04	-8.47	-8.42	CaCO3
CaSeO3	-5.64	-11.24	-5.60	CaSeO3
Cd(gamma)	-31.31	-17.19	14.13	Cd
Cd(OH)2	-7.54	6.11	13.65	Cd(OH)2
Cd(OH)2(a)	-8.23	6.11	14.35	Cd(OH)2
Cd3(OH)2(SO4)2	-25.70	-18.99	6.71	Cd3(OH)2(SO4)2
Cd3(OH)4SO4	-22.88	-0.32	22.56	Cd3(OH)4SO4
Cd4(OH)6SO4	-22.61	5.79	28.40	Cd4(OH)6SO4
CdCl2	-15.44	-15.99	-0.55	CdCl2
CdCl2:2.5H2O	-14.00	-15.99	-1.99	CdCl2:2.5H2O
CdCl2:H2O	-14.33	-15.99	-1.66	CdCl2:H2O
CdMetal	-31.21	-17.19	14.02	Cd
CdOHCl	-8.68	-4.94	3.74	CdOHCl
CdSiO3	-6.87	2.68	9.55	CdSiO3
CdSO4	-12.89	-12.55	0.34	CdSO4
CdSO4:2.7H2O	-10.81	-12.55	-1.75	CdSO4:2.67H2O
CdSO4:H2O	-11.12	-12.55	-1.43	CdSO4:H2O
Cerrusite	-3.12	-16.40	-13.27	PbCO3
Chalcanthite	-10.12	-12.80	-2.68	CuSO4:5H2O
Chalcedony	0.26	-3.43	-3.69	SiO2
Chrysotile	-6.09	27.60	33.69	Mg3Si2O5(OH)4

Claudetite	-32.25	-33.79	-1.54	As2O3
Clinoenstatite	-3.88	8.06	11.94	MgSiO3
CO2(g)	-2.57	-3.89	-1.32	CO2
Coffinite	-7.55	-14.88	-7.33	USiO4
Cotunnite	-12.79	-17.73	-4.94	PbCl2
Cristobalite	0.32	-3.43	-3.75	SiO2
Cu(OH)2	-3.22	5.87	9.09	Cu(OH)2
Cu2SO4	-23.07	-24.89	-1.81	Cu2SO4
Cu3(AsO4)2:6w	-17.36	-52.48	-35.12	Cu3(AsO4)2:6H2O
CuCO3	-5.27	-14.90	-9.63	CuCO3
CuMetal	-5.49	-14.76	-9.27	Cu
CuOCuSO4	-19.52	-6.93	12.59	CuO:CuSO4
CupricFerrite	12.11	19.14	7.03	CuFe2O4
Cuprite	-4.49	-6.22	-1.74	Cu2O
CuprousFerrite	12.33	3.52	-8.81	CuFeO2
CuSO4	-16.35	-12.80	3.55	CuSO4
Diopside	-3.92	16.93	20.85	CaMgSi2O6
Dioptase	-4.33	2.44	6.77	CuSiO3:H2O
Dolomite	-0.94	-17.75	-16.81	CaMg(CO3)2
Dolomite(d)	-1.54	-17.75	-16.21	CaMg(CO3)2
Epsomite	-4.96	-7.18	-2.22	MgSO4:7H2O
Fe(OH)2.7Cl.3	6.36	3.32	-3.04	Fe(OH)2.7Cl0.3
Fe(OH)3(a)	1.74	6.63	4.89	Fe(OH)3
Fe2(SeO3)3	-21.94	-57.37	-35.43	Fe2(SeO3)3
Fe3(OH)8	1.34	21.56	20.22	Fe3(OH)8
FeSe2	-51.69	-70.27	-18.58	FeSe2
Forsterite	-10.20	19.55	29.75	Mg2SiO4
Goethite	7.20	6.63	-0.57	FeOOH
Goslarite	-7.40	-9.46	-2.06	ZnSO4:7H2O
Greenalite	-2.80	18.01	20.81	Fe3Si2O5(OH)4
Gummite	-9.29	1.79	11.09	UO3
Gypsum	-1.78	-6.36	-4.59	CaSO4:2H2O
H2(g)	-23.30	-26.40	-3.10	H2
H2O(g)	-1.82	-0.00	1.82	H2O
Halite	-7.77	-6.21	1.55	NaCl
Hausmannite	-14.05	49.97	64.02	Mn3O4
Hematite	16.36	13.27	-3.09	Fe2O3
Huntite	-7.12	-36.32	-29.20	CaMg3(CO3)4
Hydrocerrusite	-10.96	-28.42	-17.46	Pb(OH)2:2PbCO3
Hydromagnesite	-18.44	-25.65	-7.21	Mg5(CO3)4(OH)2:4H2O
Jarosite(ss)	-4.77	-14.60	-9.83	(K0.77Na0.03H0.2)Fe3(SO4)2(OH)6
Jarosite-K	-5.66	-13.95	-8.28	KFe3(SO4)2(OH)6
Jarosite-Na	-8.38	-12.59	-4.21	NaFe3(SO4)2(OH)6
JarositeH	-13.68	-17.43	-3.75	(H3O)Fe3(SO4)2(OH)6
Langite	-13.16	4.81	17.97	Cu4(OH)6SO4:H2O
Larnakite	-9.83	-9.92	-0.09	PbO:PbSO4
Laurionite	-7.30	-6.68	0.62	PbOHCl
Litharge	-8.83	4.38	13.21	PbO
Magadiite	-4.87	-19.17	-14.30	NaSi7O13(OH)3:3H2O
Maghemite	6.88	13.27	6.39	Fe2O3
Magnesite	-1.44	-9.28	-7.85	MgCO3
Magnetite	16.32	21.56	5.23	Fe3O4
Malachite	-4.33	1.41	5.74	Cu2(OH)2CO3
Manganite	-4.80	20.54	25.34	MnOOH
Massicot	-9.03	4.38	13.41	PbO
Melanothallite	-20.33	-16.24	4.10	CuCl2
Melanterite	-8.01	-10.38	-2.36	FeSO4:7H2O
Minium	-40.31	36.43	76.74	Pb3O4
Mirabilite	-7.31	-8.98	-1.68	Na2SO4:10H2O
Mn2(SO4)3	-62.92	-67.47	-4.55	Mn2(SO4)3
Mn3(AsO4)2:8H2O	-14.71	-43.41	-28.71	Mn3(AsO4)2:8H2O
MnCl2:4H2O	-15.41	-13.21	2.19	MnCl2:4H2O
MnSO4	-12.91	-9.78	3.13	MnSO4
Monteponite	-8.39	6.11	14.50	CdO
Morenosite	-10.00	-12.45	-2.45	NiSO4:7H2O
Na4UO2(CO3)3	-24.87	-41.16	-16.29	Na4UO2(CO3)3
Nahcolite	-4.82	-5.48	-0.66	NaHCO3
Nantokite	-7.11	-14.16	-7.06	CuCl

Natron	-9.31	-11.09	-1.78	Na2CO3:10H2O
Nesquehonite	-3.83	-9.28	-5.45	MgCO3:3H2O
Ni(OH)2	-3.68	6.22	9.90	Ni(OH)2
Ni2SiO4	-6.52	9.01	15.53	Ni2SiO4
Ni3(AsO4)2:8H2O	-25.91	-51.42	-25.51	Ni3(AsO4)2:8H2O
Ni4(OH)6SO4	-25.78	6.22	32.00	Ni4(OH)6SO4
NiCO3	-8.01	-14.55	-6.55	NiCO3
Nsutite	-10.37	32.19	42.56	MnO2
O2(g)	-0.89	-3.68	-2.80	O2
Otavite	-2.56	-14.66	-12.10	CdCO3
Pb(OH)2	-4.19	4.38	8.57	Pb(OH)2
Pb2(OH)3Cl	-11.09	-2.30	8.79	Pb2(OH)3Cl
Pb2O(OH)2	-17.45	8.75	26.20	PbO:Pb(OH)2
Pb2O3	-28.99	32.05	61.04	Pb2O3
Pb2OCO3	-11.86	-12.02	-0.16	PbO:PbCO3
Pb2SiO4	-15.21	5.32	20.53	Pb2SiO4
Pb3(AsO4)2	-21.55	-56.96	-35.40	Pb3(AsO4)2
Pb3O2CO3	-19.45	-7.65	11.80	PbCO3:2PbO
Pb3O2SO4	-16.56	-5.54	11.02	PbSO4:2PbO
Pb4(OH)6SO4	-22.27	-1.17	21.10	Pb4(OH)6SO4
Pb4O3SO4	-24.31	-1.17	23.14	PbSO4:3PbO
PbMetal	-23.18	-18.92	4.26	Pb
PbO:0.3H2O	-8.60	4.38	12.98	PbO:0.33H2O
PbSiO3	-6.65	0.95	7.59	PbSiO3
Phosgenite	-14.32	-34.13	-19.81	PbCl2:PbCO3
Plattnerite	-23.72	27.68	51.40	PbO2
Portlandite	-11.42	12.30	23.72	Ca(OH)2
Pyrochroite	-6.31	8.89	15.20	Mn(OH)2
Pyrolusite	-11.12	32.19	43.31	MnO2
Quartz	0.73	-3.43	-4.16	SiO2
Retgersite	-10.37	-12.45	-2.07	NiSO4:6H2O
Rhodochrosite	-0.79	-11.88	-11.09	MnCO3
Rhodochrosite(d)	-1.49	-11.88	-10.39	MnCO3
Rutherfordine	-4.57	-18.98	-14.41	UO2CO3
Schoepite	-3.97	1.79	5.76	UO2(OH)2:H2O
Scorodite	-8.16	-28.41	-20.25	FeAsO4:2H2O
Se(s)	-10.31	-27.63	-17.32	Se
SeO2	-15.17	-23.55	-8.38	SeO2
Sepiolite	-3.39	12.69	16.08	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-5.97	12.69	18.66	Mg2Si3O7.5OH:3H2O
Siderite	-1.66	-12.48	-10.82	FeCO3
Siderite(d)(3)	-2.03	-12.48	-10.45	FeCO3
Silicagel	-0.28	-3.43	-3.15	SiO2
SiO2(a)	-0.62	-3.43	-2.81	SiO2
Smithsonite	-1.69	-11.56	-9.87	ZnCO3
Talc	-2.03	20.74	22.77	Mg3Si4O10(OH)2
Tenorite	-2.20	5.87	8.07	CuO
Thenardite	-8.82	-8.98	-0.16	Na2SO4
Thermonatrite	-11.30	-11.09	0.21	Na2CO3:H2O
Tremolite	-4.84	54.61	59.45	Ca2Mg5Si8O22(OH)2
Trona	-16.31	-16.57	-0.26	NaHCO3:Na2CO3:2H2O
U(OH)2SO4	-26.91	-30.11	-3.20	U(OH)2SO4
U3O8(c)	-11.71	12.26	23.97	U3O8
U4O9(c)	-22.10	-22.48	-0.38	U4O9
UO2(a)	-11.55	-11.45	0.10	UO2
UO3(gamma)	-6.50	1.79	8.29	UO3
Uraninite(c)	-7.20	-11.45	-4.25	UO2
Uranophane	-8.46	9.03	17.49	Ca(UO2)2(SiO3OH)2
Willemite	-1.33	14.99	16.32	Zn2SiO4
Witherite	-3.28	-11.89	-8.61	BaCO3
Zincite(c)	-2.58	9.21	11.79	ZnO
Zincosite	-13.04	-9.46	3.58	ZnSO4
Zn(OH)2-a	-3.24	9.21	12.45	Zn(OH)2
Zn(OH)2-b	-2.54	9.21	11.75	Zn(OH)2
Zn(OH)2-c	-2.99	9.21	12.20	Zn(OH)2
Zn(OH)2-e	-2.29	9.21	11.50	Zn(OH)2
Zn(OH)2-g	-2.50	9.21	11.71	Zn(OH)2
Zn2(OH)2SO4	-7.75	-0.25	7.50	Zn2(OH)2SO4

```
  Zn2(OH)3Cl       -7.84      7.36   15.20  Zn2(OH)3Cl
  Zn3(AsO4)2:2.5w -14.91    -42.46  -27.55  Zn3(AsO4)2:2.5H2O
  Zn3O(SO4)2      -30.57     -9.71   20.86  ZnO:2ZnSO4
  Zn4(OH)6SO4     -10.24     18.16   28.40  Zn4(OH)6SO4
  Zn5(OH)8Cl2     -14.57     23.93   38.50  Zn5(OH)8Cl2
  ZnCl2           -20.45    -12.90    7.55  ZnCl2
  ZnCO3:H2O        -1.30    -11.56  -10.26  ZnCO3:H2O
  ZnMetal         -40.94    -14.09   26.85  Zn
  ZnO(a)           -2.10      9.21   11.31  ZnO
  ZnSiO3            2.31      5.78    3.47  ZnSiO3
  ZnSO4:H2O        -9.20     -9.46   -0.25  ZnSO4:H2O

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
  For ideal gases, phi = 1.

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End of simulation.
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Reading input data for simulation 2.
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End of Run after 0.11 Seconds.
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```

```
   Input file: E:\Project Stuff\Models\Trace Metal_Inputst.pqi
  Output file: E:\Project Stuff\Models\Trace Metal_Inputst.pqo
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.1.2-8538\database
\wateq4f.dat

------------------
Reading data base.
------------------

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

      DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 3.1.2-8538\database
\wateq4f.dat
      TITLE Professional Project Geochemical Model
      SOLUTION   Pow Wow Well
              units   ppm
              pH      9.69
              temp    15.5
              O(0)            1.6
              Ca              3.58
              Mg              0.033
              Na              80.7
              K               0.635
              Ba              0.00247
              Cd              0
              Cu              0
              Zn              0.00845
              Pb              0.00148
              Mn              0
              Se              0.0032
              Ni              0.000226
              Fe              0.0124
              Al              0.0148
              U               0.024
              As              0.00956
              Cl              11.3
              Alkalinity      116.0 as HCO3
              S(6)            42.8
              Si              19.8
      END
-----
TITLE
-----

 Professional Project Geochemical Model

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

Initial solution 1.     Pow Wow Well

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

      Elements           Molality       Moles

      Al                5.487e-07   5.487e-07
```

Alkalinity	1.902e-03	1.902e-03
As	1.276e-07	1.276e-07
Ba	1.799e-08	1.799e-08
Ca	8.935e-05	8.935e-05
Cl	3.188e-04	3.188e-04
Fe	2.221e-07	2.221e-07
K	1.624e-05	1.624e-05
Mg	1.358e-06	1.358e-06
Na	3.511e-03	3.511e-03
Ni	3.850e-09	3.850e-09
O(0)	1.000e-04	1.000e-04
Pb	7.145e-09	7.145e-09
S(6)	4.457e-04	4.457e-04
Se	4.054e-08	4.054e-08
Si	3.296e-04	3.296e-04
U	1.009e-07	1.009e-07
Zn	1.293e-07	1.293e-07

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

pH	= 9.690
pe	= 4.000
Activity of water	= 1.000
Ionic strength	= 4.129e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 1.468e-03
Total CO2 (mol/kg)	= 1.468e-03
Temperature (°C)	= 15.50
Electrical balance (eq)	= 5.993e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 8.93
Iterations	= 13
Total H	= 1.110148e+02
Total O	= 5.551385e+01

----------Redox couples----------

Redox couple	pe	Eh (volts)
O(-2)/O(0)	11.5678	0.6625

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	2.467e-05	2.302e-05	-4.608	-4.638	-0.030	(0)
H+	2.173e-10	2.042e-10	-9.663	-9.690	-0.027	0.00
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.03
Al	5.487e-07					
Al(OH)4-	5.486e-07	5.126e-07	-6.261	-6.290	-0.029	(0)
Al(OH)3	6.148e-11	6.154e-11	-10.211	-10.211	0.000	(0)
Al(OH)2+	1.922e-13	1.798e-13	-12.716	-12.745	-0.029	(0)
AlOH+2	1.472e-17	1.127e-17	-16.832	-16.948	-0.116	(0)
Al+3	7.641e-22	4.355e-22	-21.117	-21.361	-0.244	(0)
AlSO4+	4.331e-22	4.047e-22	-21.363	-21.393	-0.029	(0)
Al(SO4)2-	4.367e-24	4.080e-24	-23.360	-23.389	-0.029	(0)
AlHSO4+2	8.964e-33	6.819e-33	-32.047	-32.166	-0.119	(0)
As(3)	1.913e-24					
H2AsO3-	1.379e-24	1.288e-24	-23.861	-23.890	-0.030	(0)
H3AsO3	5.347e-25	5.352e-25	-24.272	-24.271	0.000	(0)
HAsO3-2	1.083e-29	8.242e-30	-28.965	-29.084	-0.119	(0)
H4AsO3+	5.798e-35	5.414e-35	-34.237	-34.266	-0.030	(0)
AsO3-3	1.065e-35	5.755e-36	-34.973	-35.240	-0.267	(0)
As(5)	1.276e-07					
HAsO4-2	1.258e-07	9.569e-08	-6.900	-7.019	-0.119	(0)
AsO4-3	1.525e-09	8.240e-10	-8.817	-9.084	-0.267	(0)
H2AsO4-	3.156e-10	2.947e-10	-9.501	-9.531	-0.030	(0)
H3AsO4	1.092e-17	1.093e-17	-16.962	-16.961	0.000	(0)

Ba	1.799e-08					
Ba+2	1.498e-08	1.145e-08	-7.824	-7.941	-0.117	(0)
BaSO4	1.914e-09	1.915e-09	-8.718	-8.718	0.000	(0)
BaCO3	9.934e-10	9.943e-10	-9.003	-9.002	0.000	(0)
BaHCO3+	9.583e-11	8.950e-11	-10.018	-10.048	-0.030	(0)
BaOH+	2.032e-12	1.900e-12	-11.692	-11.721	-0.029	(0)
C(4)	1.468e-03					
HCO3-	1.175e-03	1.100e-03	-2.930	-2.959	-0.029	(0)
CO3-2	2.656e-04	2.034e-04	-3.576	-3.692	-0.116	(0)
CaCO3	1.558e-05	1.559e-05	-4.807	-4.807	0.000	(0)
NaCO3-	8.062e-06	7.542e-06	-5.094	-5.123	-0.029	(0)
NaHCO3	2.018e-06	2.020e-06	-5.695	-5.695	0.000	(0)
CaHCO3+	6.699e-07	6.271e-07	-6.174	-6.203	-0.029	(0)
CO2	5.829e-07	5.835e-07	-6.234	-6.234	0.000	(0)
MgCO3	1.466e-07	1.467e-07	-6.834	-6.833	0.000	(0)
UO2(CO3)3-4	9.439e-08	3.161e-08	-7.025	-7.500	-0.475	(0)
Zn(CO3)2-2	5.141e-08	3.911e-08	-7.289	-7.408	-0.119	(0)
MgHCO3+	1.167e-08	1.089e-08	-7.933	-7.963	-0.030	(0)
ZnCO3	8.985e-09	8.993e-09	-8.047	-8.046	0.000	(0)
PbCO3	4.068e-09	4.072e-09	-8.391	-8.390	0.000	(0)
Pb(CO3)2-2	2.735e-09	2.080e-09	-8.563	-8.682	-0.119	(0)
NiCO3	2.623e-09	2.625e-09	-8.581	-8.581	0.000	(0)
UO2(CO3)2-2	2.256e-09	1.716e-09	-8.647	-8.765	-0.119	(0)
Ni(CO3)2-2	1.220e-09	9.280e-10	-8.914	-9.032	-0.119	(0)
BaCO3	9.934e-10	9.943e-10	-9.003	-9.002	0.000	(0)
BaHCO3+	9.583e-11	8.950e-11	-10.018	-10.048	-0.030	(0)
ZnHCO3+	3.284e-11	3.067e-11	-10.484	-10.513	-0.030	(0)
PbHCO3+	1.077e-12	1.006e-12	-11.968	-11.997	-0.030	(0)
UO2CO3	4.300e-13	4.304e-13	-12.366	-12.366	0.000	(0)
NiHCO3+	2.830e-13	2.643e-13	-12.548	-12.578	-0.030	(0)
FeCO3	5.637e-14	5.643e-14	-13.249	-13.249	0.000	(0)
FeHCO3+	1.362e-15	1.272e-15	-14.866	-14.896	-0.030	(0)
(UO2)3(CO3)6-6	1.238e-22	1.056e-23	-21.907	-22.976	-1.069	(0)
UO2(CO3)3-5	2.047e-24	3.706e-25	-23.689	-24.431	-0.742	(0)
U(CO3)4-4	2.778e-37	9.303e-38	-36.556	-37.031	-0.475	(0)
U(CO3)5-6	9.193e-40	0.000e+00	-39.037	-40.106	-1.069	(0)
Ca	8.935e-05					
Ca+2	6.981e-05	5.343e-05	-4.156	-4.272	-0.116	(0)
CaCO3	1.558e-05	1.559e-05	-4.807	-4.807	0.000	(0)
CaSO4	3.243e-06	3.246e-06	-5.489	-5.489	0.000	(0)
CaHCO3+	6.699e-07	6.271e-07	-6.174	-6.203	-0.029	(0)
CaOH+	4.639e-08	4.343e-08	-7.334	-7.362	-0.029	(0)
CaHSO4+	3.735e-15	3.488e-15	-14.428	-14.457	-0.030	(0)
Cl	3.188e-04					
Cl-	3.188e-04	2.975e-04	-3.496	-3.526	-0.030	(0)
ZnOHCl	1.068e-11	1.069e-11	-10.971	-10.971	0.000	(0)
ZnCl+	1.233e-13	1.151e-13	-12.909	-12.939	-0.030	(0)
PbCl+	1.146e-14	1.070e-14	-13.941	-13.971	-0.030	(0)
NiCl+	1.393e-15	1.301e-15	-14.856	-14.886	-0.030	(0)
ZnCl2	3.445e-17	3.448e-17	-16.463	-16.462	0.000	(0)
PbCl2	6.054e-18	6.060e-18	-17.218	-17.218	0.000	(0)
FeCl+	5.080e-18	4.750e-18	-17.294	-17.323	-0.029	(0)
NiCl2	1.405e-18	1.406e-18	-17.852	-17.852	0.000	(0)
ZnCl3-	1.162e-20	1.085e-20	-19.935	-19.964	-0.030	(0)
PbCl3-	1.444e-21	1.348e-21	-20.841	-20.870	-0.030	(0)
UO2Cl+	2.249e-22	2.100e-22	-21.648	-21.678	-0.030	(0)
ZnCl4-2	1.960e-24	1.498e-24	-23.708	-23.825	-0.117	(0)
PbCl4-2	2.340e-25	1.780e-25	-24.631	-24.750	-0.119	(0)
FeCl+2	5.557e-26	4.247e-26	-25.255	-25.372	-0.117	(0)
UO2Cl2	3.050e-27	3.053e-27	-26.516	-26.515	0.000	(0)
FeCl2+	8.249e-29	7.704e-29	-28.084	-28.113	-0.030	(0)
FeCl3	2.290e-33	2.292e-33	-32.640	-32.640	0.000	(0)
UCl+3	0.000e+00	0.000e+00	-56.594	-56.862	-0.267	(0)
Fe(2)	8.275e-14					
FeCO3	5.637e-14	5.643e-14	-13.249	-13.249	0.000	(0)
Fe+2	1.506e-14	1.156e-14	-13.822	-13.937	-0.115	(0)
FeOH+	9.202e-15	8.603e-15	-14.036	-14.065	-0.029	(0)
FeHCO3+	1.362e-15	1.272e-15	-14.866	-14.896	-0.030	(0)

FeSO4	5.731e-16	5.736e-16	-15.242	-15.241	0.000	(0)
Fe(OH)2	1.526e-16	1.527e-16	-15.816	-15.816	0.000	(0)
Fe(OH)3-	2.699e-17	2.524e-17	-16.569	-16.598	-0.029	(0)
FeCl+	5.080e-18	4.750e-18	-17.294	-17.323	-0.029	(0)
FeHSO4+	8.084e-25	7.549e-25	-24.092	-24.122	-0.030	(0)
Fe(3)	2.221e-07					
Fe(OH)4-	1.694e-07	1.584e-07	-6.771	-6.800	-0.029	(0)
Fe(OH)3	5.258e-08	5.263e-08	-7.279	-7.279	0.000	(0)
Fe(OH)2+	1.368e-10	1.279e-10	-9.864	-9.893	-0.029	(0)
FeOH+2	1.498e-16	1.145e-16	-15.825	-15.941	-0.117	(0)
FeSO4+	2.032e-23	1.900e-23	-22.692	-22.721	-0.029	(0)
Fe+3	1.132e-23	6.451e-24	-22.946	-23.190	-0.244	(0)
Fe(SO4)2-	1.429e-25	1.335e-25	-24.845	-24.875	-0.030	(0)
FeCl+2	5.557e-26	4.247e-26	-25.255	-25.372	-0.117	(0)
FeCl2+	8.249e-29	7.704e-29	-28.084	-28.113	-0.030	(0)
Fe2(OH)2+4	1.580e-30	5.290e-31	-29.801	-30.277	-0.475	(0)
FeHSO4+2	1.390e-32	1.058e-32	-31.857	-31.976	-0.119	(0)
FeCl3	2.290e-33	2.292e-33	-32.640	-32.640	0.000	(0)
Fe3(OH)4+5	1.932e-37	3.497e-38	-36.714	-37.456	-0.742	(0)
H(0)	6.502e-31					
H2	3.251e-31	3.254e-31	-30.488	-30.488	0.000	(0)
K	1.624e-05					
K+	1.621e-05	1.513e-05	-4.790	-4.820	-0.030	(0)
KSO4-	3.196e-08	2.990e-08	-7.495	-7.524	-0.029	(0)
Mg	1.358e-06					
Mg+2	1.140e-06	8.747e-07	-5.943	-6.058	-0.115	(0)
MgCO3	1.466e-07	1.467e-07	-6.834	-6.833	0.000	(0)
MgSO4	5.310e-08	5.315e-08	-7.275	-7.275	0.000	(0)
MgHCO3+	1.167e-08	1.089e-08	-7.933	-7.963	-0.030	(0)
MgOH+	6.845e-09	6.412e-09	-8.165	-8.193	-0.028	(0)
Na	3.511e-03					
Na+	3.496e-03	3.266e-03	-2.456	-2.486	-0.029	(0)
NaCO3-	8.062e-06	7.542e-06	-5.094	-5.123	-0.029	(0)
NaSO4-	5.488e-06	5.134e-06	-5.261	-5.290	-0.029	(0)
NaHCO3	2.018e-06	2.020e-06	-5.695	-5.695	0.000	(0)
Ni	3.850e-09					
NiCO3	2.623e-09	2.625e-09	-8.581	-8.581	0.000	(0)
Ni(CO3)2-2	1.220e-09	9.280e-10	-8.914	-9.032	-0.119	(0)
Ni(OH)2	4.172e-12	4.176e-12	-11.380	-11.379	0.000	(0)
Ni+2	2.289e-12	1.741e-12	-11.640	-11.759	-0.119	(0)
NiOH+	6.322e-13	5.904e-13	-12.199	-12.229	-0.030	(0)
NiHCO3+	2.830e-13	2.643e-13	-12.548	-12.578	-0.030	(0)
Ni(OH)3-	2.190e-13	2.045e-13	-12.660	-12.689	-0.030	(0)
NiSO4	1.040e-13	1.041e-13	-12.983	-12.982	0.000	(0)
NiCl+	1.393e-15	1.301e-15	-14.856	-14.886	-0.030	(0)
Ni(SO4)2-2	2.669e-18	2.031e-18	-17.574	-17.692	-0.119	(0)
NiCl2	1.405e-18	1.406e-18	-17.852	-17.852	0.000	(0)
O(0)	1.000e-04					
O2	5.001e-05	5.006e-05	-4.301	-4.300	0.000	(0)
Pb	7.145e-09					
PbCO3	4.068e-09	4.072e-09	-8.391	-8.390	0.000	(0)
Pb(CO3)2-2	2.735e-09	2.080e-09	-8.563	-8.682	-0.119	(0)
Pb(OH)2	2.094e-10	2.096e-10	-9.679	-9.679	0.000	(0)
PbOH+	1.178e-10	1.100e-10	-9.929	-9.959	-0.030	(0)
Pb(OH)3-	1.262e-11	1.178e-11	-10.899	-10.929	-0.030	(0)
Pb+2	1.514e-12	1.152e-12	-11.820	-11.939	-0.119	(0)
PbHCO3+	1.077e-12	1.006e-12	-11.968	-11.997	-0.030	(0)
PbSO4	2.160e-13	2.162e-13	-12.666	-12.665	0.000	(0)
Pb(OH)4-2	1.738e-13	1.322e-13	-12.760	-12.879	-0.119	(0)
PbCl+	1.146e-14	1.070e-14	-13.941	-13.971	-0.030	(0)
Pb(SO4)2-2	4.977e-16	3.786e-16	-15.303	-15.422	-0.119	(0)
PbCl2	6.054e-18	6.060e-18	-17.218	-17.218	0.000	(0)
Pb2OH+3	5.248e-21	2.837e-21	-20.280	-20.547	-0.267	(0)
PbCl3-	1.444e-21	1.348e-21	-20.841	-20.870	-0.030	(0)
Pb3(OH)4+2	3.496e-22	2.659e-22	-21.456	-21.575	-0.119	(0)
PbCl4-2	2.340e-25	1.780e-25	-24.631	-24.750	-0.119	(0)
S(6)	4.457e-04					
SO4-2	4.369e-04	3.337e-04	-3.360	-3.477	-0.117	(0)

NaSO4-	5.488e-06	5.134e-06	-5.261	-5.290	-0.029	(0)
CaSO4	3.243e-06	3.246e-06	-5.489	-5.489	0.000	(0)
MgSO4	5.310e-08	5.315e-08	-7.275	-7.275	0.000	(0)
KSO4-	3.196e-08	2.990e-08	-7.495	-7.524	-0.029	(0)
BaSO4	1.914e-09	1.915e-09	-8.718	-8.718	0.000	(0)
ZnSO4	1.606e-11	1.607e-11	-10.794	-10.794	0.000	(0)
HSO4-	5.811e-12	5.430e-12	-11.236	-11.265	-0.029	(0)
PbSO4	2.160e-13	2.162e-13	-12.666	-12.665	0.000	(0)
NiSO4	1.040e-13	1.041e-13	-12.983	-12.982	0.000	(0)
Zn(SO4)2-2	6.182e-14	4.702e-14	-13.209	-13.328	-0.119	(0)
CaHSO4+	3.735e-15	3.488e-15	-14.428	-14.457	-0.030	(0)
FeSO4	5.731e-16	5.736e-16	-15.242	-15.241	0.000	(0)
Pb(SO4)2-2	4.977e-16	3.786e-16	-15.303	-15.422	-0.119	(0)
Ni(SO4)2-2	2.669e-18	2.031e-18	-17.574	-17.692	-0.119	(0)
UO2SO4	1.924e-19	1.925e-19	-18.716	-18.715	0.000	(0)
UO2(SO4)2-2	6.721e-22	5.113e-22	-21.173	-21.291	-0.119	(0)
AlSO4+	4.331e-22	4.047e-22	-21.363	-21.393	-0.029	(0)
FeSO4+	2.032e-23	1.900e-23	-22.692	-22.721	-0.029	(0)
Al(SO4)2-	4.367e-24	4.080e-24	-23.360	-23.389	-0.029	(0)
FeHSO4+	8.084e-25	7.549e-25	-24.092	-24.122	-0.030	(0)
Fe(SO4)2-	1.429e-25	1.335e-25	-24.845	-24.875	-0.030	(0)
FeHSO4+2	1.390e-32	1.058e-32	-31.857	-31.976	-0.119	(0)
AlHSO4+2	8.964e-33	6.819e-33	-32.047	-32.166	-0.119	(0)
U(SO4)2	0.000e+00	0.000e+00	-51.807	-51.806	0.000	(0)
USO4+2	0.000e+00	0.000e+00	-51.988	-52.107	-0.119	(0)
Se(-2)	0.000e+00					
HSe-	0.000e+00	0.000e+00	-56.820	-56.850	-0.030	(0)
H2Se	0.000e+00	0.000e+00	-62.612	-62.612	0.000	(0)
Se(4)	4.049e-08					
SeO3-2	3.846e-08	2.926e-08	-7.415	-7.534	-0.119	(0)
HSeO3-	2.023e-09	1.889e-09	-8.694	-8.724	-0.030	(0)
H2SeO3	2.167e-16	2.169e-16	-15.664	-15.664	0.000	(0)
Se(6)	5.117e-11					
SeO4-2	5.117e-11	3.893e-11	-10.291	-10.410	-0.119	(0)
HSeO4-	2.961e-19	2.766e-19	-18.529	-18.558	-0.030	(0)
Si	3.296e-04					
H4SiO4	2.134e-04	2.136e-04	-3.671	-3.670	0.000	(0)
H3SiO4-	1.162e-04	1.085e-04	-3.935	-3.965	-0.030	(0)
H2SiO4-2	2.453e-08	1.878e-08	-7.610	-7.726	-0.116	(0)
U(3)	0.000e+00					
U+3	0.000e+00	0.000e+00	-68.282	-68.549	-0.267	(0)
U(4)	3.157e-26					
U(OH)4	3.157e-26	3.160e-26	-25.501	-25.500	0.000	(0)
U(OH)3+	2.841e-32	2.653e-32	-31.547	-31.576	-0.030	(0)
U(CO3)4-4	2.778e-37	9.303e-38	-36.556	-37.031	-0.475	(0)
U(OH)2+2	4.327e-39	3.291e-39	-38.364	-38.483	-0.119	(0)
U(CO3)5-6	9.193e-40	0.000e+00	-39.037	-40.106	-1.069	(0)
UOH+3	0.000e+00	0.000e+00	-46.018	-46.285	-0.267	(0)
U(SO4)2	0.000e+00	0.000e+00	-51.807	-51.806	0.000	(0)
USO4+2	0.000e+00	0.000e+00	-51.988	-52.107	-0.119	(0)
U+4	0.000e+00	0.000e+00	-54.690	-55.165	-0.475	(0)
UCl+3	0.000e+00	0.000e+00	-56.594	-56.862	-0.267	(0)
U6(OH)15+9	0.000e+00	0.000e+00	-200.434	-202.840	-2.405	(0)
U(5)	2.110e-21					
UO2+	2.108e-21	1.968e-21	-20.676	-20.706	-0.030	(0)
UO2(CO3)3-5	2.047e-24	3.706e-25	-23.689	-24.431	-0.742	(0)
U(6)	1.009e-07					
UO2(CO3)3-4	9.439e-08	3.161e-08	-7.025	-7.500	-0.475	(0)
UO2(OH)3-	4.208e-09	3.930e-09	-8.376	-8.406	-0.030	(0)
UO2(CO3)2-2	2.256e-09	1.716e-09	-8.647	-8.765	-0.119	(0)
UO2CO3	4.300e-13	4.304e-13	-12.366	-12.366	0.000	(0)
UO2(OH)4-2	4.010e-13	3.050e-13	-12.397	-12.516	-0.119	(0)
UO2OH+	9.516e-15	8.887e-15	-14.022	-14.051	-0.030	(0)
(UO2)3(OH)7-	1.079e-18	1.007e-18	-17.967	-17.997	-0.030	(0)
UO2+2	6.971e-19	5.303e-19	-18.157	-18.275	-0.119	(0)
UO2SO4	1.924e-19	1.925e-19	-18.716	-18.715	0.000	(0)
UO2(SO4)2-2	6.721e-22	5.113e-22	-21.173	-21.291	-0.119	(0)
UO2Cl+	2.249e-22	2.100e-22	-21.648	-21.678	-0.030	(0)

(UO2)3(CO3)6-6	1.238e-22	1.056e-23	-21.907	-22.976	-1.069	(0)
(UO2)3(OH)5+	3.148e-23	2.940e-23	-22.502	-22.532	-0.030	(0)
(UO2)2(OH)2+2	1.205e-23	9.165e-24	-22.919	-23.038	-0.119	(0)
UO2Cl2	3.050e-27	3.053e-27	-26.516	-26.515	0.000	(0)
(UO2)4(OH)7+	7.202e-28	6.726e-28	-27.143	-27.172	-0.030	(0)
(UO2)3(OH)4+2	1.419e-28	1.080e-28	-27.848	-27.967	-0.119	(0)
(UO2)2OH+3	5.084e-30	2.748e-30	-29.294	-29.561	-0.267	(0)
Zn	1.293e-07					
Zn(OH)2	6.684e-08	6.691e-08	-7.175	-7.175	0.000	(0)
Zn(CO3)2-2	5.141e-08	3.911e-08	-7.289	-7.408	-0.119	(0)
ZnCO3	8.985e-09	8.993e-09	-8.047	-8.046	0.000	(0)
Zn(OH)3-	1.109e-09	1.036e-09	-8.955	-8.985	-0.030	(0)
ZnOH+	6.053e-10	5.653e-10	-9.218	-9.248	-0.030	(0)
Zn+2	2.885e-10	2.216e-10	-9.540	-9.654	-0.115	(0)
ZnHCO3+	3.284e-11	3.067e-11	-10.484	-10.513	-0.030	(0)
ZnSO4	1.606e-11	1.607e-11	-10.794	-10.794	0.000	(0)
ZnOHCl	1.068e-11	1.069e-11	-10.971	-10.971	0.000	(0)
Zn(OH)4-2	1.057e-12	8.042e-13	-11.976	-12.095	-0.119	(0)
ZnCl+	1.233e-13	1.151e-13	-12.909	-12.939	-0.030	(0)
Zn(SO4)2-2	6.182e-14	4.702e-14	-13.209	-13.328	-0.119	(0)
ZnCl2	3.445e-17	3.448e-17	-16.463	-16.462	0.000	(0)
ZnCl3-	1.162e-20	1.085e-20	-19.935	-19.964	-0.030	(0)
ZnCl4-2	1.960e-24	1.498e-24	-23.708	-23.825	-0.117	(0)

----------Saturation indices----------

Phase	SI**	log IAP	log K(288 K, 1 atm)	
Adularia	-0.80	-22.12	-21.32	KAlSi3O8
Al(OH)3(a)	-3.73	7.71	11.44	Al(OH)3
AlAsO4:2H2O	-14.61	-30.45	-15.84	AlAsO4:2H2O
Albite	-1.16	-19.79	-18.63	NaAlSi3O8
AlumK	-27.79	-33.13	-5.34	KAl(SO4)2:12H2O
Alunite	-17.53	-17.72	-0.19	KAl3(SO4)2(OH)6
Analcime	-2.98	-16.12	-13.14	NaAlSi2O6:H2O
Anglesite	-7.57	-15.42	-7.84	PbSO4
Anhydrite	-3.41	-7.75	-4.34	CaSO4
Annite	-4.61	-91.76	-87.15	KFe3AlSi3O10(OH)2
Anorthite	-4.20	-24.19	-19.99	CaAl2Si2O8
Aragonite	0.32	-7.96	-8.28	CaCO3
Arsenolite	-46.99	-48.54	-1.55	As2O3
Artinite	-6.72	3.57	10.29	MgCO3:Mg(OH)2:3H2O
As2O5(cr)	-42.33	-33.92	8.41	As2O5
As_native	-52.15	-65.34	-13.20	As
B-UO2(OH)2	-4.77	1.10	5.88	UO2(OH)2
Ba3(AsO4)2	8.35	-41.99	-50.34	Ba3(AsO4)2
Barite	-1.28	-11.42	-10.13	BaSO4
Basaluminite	-14.72	7.98	22.70	Al4(OH)10SO4
BaSeO3	-9.08	-15.47	-6.39	BaSeO3
Beidellite	-1.91	-48.64	-46.73	(NaKMg0.5)0.11Al2.33Si3.67O10(OH)2
Bianchite	-11.37	-13.13	-1.76	ZnSO4:6H2O
Boehmite	-1.55	7.71	9.26	AlOOH
Brucite	-4.17	13.32	17.49	Mg(OH)2
Bunsenite	-5.41	7.62	13.03	NiO
Ca3(AsO4)2:4w	-12.08	-30.98	-18.91	Ca3(AsO4)2:4H2O
Calcite	0.47	-7.96	-8.43	CaCO3
CaSeO3	-6.21	-11.81	-5.60	CaSeO3
Cerrusite	-2.38	-15.63	-13.25	PbCO3
Chalcedony	-0.01	-3.67	-3.67	SiO2
Chlorite14A	-1.02	71.02	72.03	Mg5Al2Si3O10(OH)8
Chlorite7A	-4.48	71.02	75.50	Mg5Al2Si3O10(OH)8
Chrysotile	-0.79	32.62	33.42	Mg3Si2O5(OH)4
Claudetite	-47.04	-48.54	-1.50	As2O3
Clinoenstatite	-2.17	9.65	11.83	MgSiO3
CO2(g)	-4.89	-6.23	-1.35	CO2
Coffinite	-12.69	-20.08	-7.39	USiO4
Cotunnite	-14.09	-18.99	-4.91	PbCl2
Cristobalite	0.05	-3.67	-3.72	SiO2

Diaspore	0.23	7.71	7.47	AlOOH
Diopside	0.41	21.09	20.67	CaMgSi2O6
Dolomite	-0.85	-17.71	-16.86	CaMg(CO3)2
Dolomite(d)	-1.44	-17.71	-16.27	CaMg(CO3)2
Epsomite	-7.33	-9.54	-2.21	MgSO4:7H2O
Fe(OH)2.7Cl.3	4.95	1.91	-3.04	Fe(OH)2.7Cl0.3
Fe(OH)3(a)	0.99	5.88	4.89	Fe(OH)3
Fe2(SeO3)3	-33.55	-68.98	-35.43	Fe2(SeO3)3
Fe3(OH)8	-3.02	17.20	20.22	Fe3(OH)8
FeSe2	-81.68	-100.26	-18.58	FeSe2
Forsterite	-6.50	22.97	29.48	Mg2SiO4
Gibbsite	-0.95	7.71	8.66	Al(OH)3
Goethite	6.53	5.88	-0.65	FeOOH
Goslarite	-11.09	-13.13	-2.04	ZnSO4:7H2O
Greenalite	-11.82	8.99	20.81	Fe3Si2O5(OH)4
Gummite	-9.85	1.10	10.96	UO3
Gypsum	-3.16	-7.75	-4.58	CaSO4:2H2O
H2(g)	-27.38	-30.49	-3.11	H2
H2O(g)	-1.76	-0.00	1.76	H2O
Halite	-7.57	-6.01	1.56	NaCl
Halloysite	-5.38	8.08	13.46	Al2Si2O5(OH)4
Hematite	15.02	11.76	-3.26	Fe2O3
Huntite	-7.87	-37.21	-29.35	CaMg3(CO3)4
Hydrocerrusite	-6.36	-23.82	-17.46	Pb(OH)2:2PbCO3
Hydromagnesite	-18.18	-25.68	-7.50	Mg5(CO3)4(OH)2:4H2O
Illite	-1.76	-43.35	-41.59	K0.6Mg0.25Al2.3Si3.5O10(OH)2
Jarosite(ss)	-14.28	-24.11	-9.83	(K0.77Na0.03H0.2)Fe3(SO4)2(OH)6
Jarosite-K	-14.75	-23.20	-8.46	KFe3(SO4)2(OH)6
Jarosite-Na	-16.46	-20.87	-4.41	NaFe3(SO4)2(OH)6
JarositeH	-24.02	-28.07	-4.06	(H3O)Fe3(SO4)2(OH)6
Jurbanite	-11.92	-15.15	-3.23	AlOHSO4
Kaolinite	-0.21	8.08	8.29	Al2Si2O5(OH)4
Kmica	2.85	16.99	14.14	KAl3Si3O10(OH)2
Larnakite	-7.85	-7.97	-0.12	PbO:PbSO4
Laumontite	0.38	-31.53	-31.92	CaAl2Si4O12:4H2O
Laurionite	-6.40	-5.78	0.62	PbOHCl
Leonhardite	8.86	-63.07	-71.93	Ca2Al4Si8O24:7H2O
Litharge	-5.67	7.44	13.12	PbO
Magadiite	-4.19	-18.49	-14.30	NaSi7O13(OH)3:3H2O
Maghemite	5.37	11.76	6.39	Fe2O3
Magnesite	-1.87	-9.75	-7.88	MgCO3
Magnetite	12.25	17.20	4.95	Fe3O4
Massicot	-5.87	7.44	13.31	PbO
Melanterite	-15.08	-17.41	-2.33	FeSO4:7H2O
Minium	-26.46	49.70	76.17	Pb3O4
Mirabilite	-6.88	-8.45	-1.57	Na2SO4:10H2O
Montmorillonite-Aberdeen	1.80	-27.89	-29.69	(HNaK)0.14Mg0.45Fe0.33Al1.47Si3.82O10(OH)2
Montmorillonite-BelleFourche	1.76	-33.15	-34.91	(HNaK)0.09Mg0.29Fe0.24Al1.57Si3.93O10(OH)2
Montmorillonite-Ca	-1.78	-48.21	-46.44	Ca0.165Al2.33Si3.67O10(OH)2
Morenosite	-12.81	-15.24	-2.43	NiSO4:7H2O
Na4UO2(CO3)3	-23.00	-39.29	-16.29	Na4UO2(CO3)3
Nahcolite	-4.81	-5.44	-0.64	NaHCO3
Natron	-6.97	-8.66	-1.69	Na2CO3:10H2O
Nesquehonite	-4.27	-9.75	-5.48	MgCO3:3H2O
Ni(OH)2	-2.44	7.62	10.07	Ni(OH)2
Ni2SiO4	-3.77	11.57	15.34	Ni2SiO4
Ni3(AsO4)2:8H2O	-27.93	-53.45	-25.51	Ni3(AsO4)2:8H2O
Ni4(OH)6SO4	-24.37	7.63	32.00	Ni4(OH)6SO4
NiCO3	-8.85	-15.45	-6.60	NiCO3
O2(g)	-1.48	-4.30	-2.82	O2
Pb(OH)2	-1.05	7.44	8.49	Pb(OH)2
Pb2(OH)3Cl	-7.13	1.67	8.79	Pb2(OH)3Cl
Pb2O(OH)2	-11.32	14.88	26.20	PbO:Pb(OH)2
Pb2O3	-18.78	42.26	61.04	Pb2O3
Pb2OCO3	-7.97	-8.19	-0.22	PbO:PbCO3
Pb2SiO4	-9.17	11.21	20.39	Pb2SiO4

Pb3(AsO4)2	-18.58	-53.98	-35.40	Pb3(AsO4)2
Pb3O2CO3	-12.41	-0.75	11.66	PbCO3:2PbO
Pb3O2SO4	-11.43	-0.53	10.90	PbSO4:2PbO
Pb4(OH)6SO4	-14.19	6.91	21.10	Pb4(OH)6SO4
Pb4O3SO4	-16.04	6.91	22.95	PbSO4:3PbO
PbMetal	-24.20	-19.94	4.26	Pb
PbO:0.3H2O	-5.54	7.44	12.98	PbO:0.33H2O
PbSiO3	-3.77	3.77	7.54	PbSiO3
Phillipsite	-1.08	-20.95	-19.87	Na0.5K0.5AlSi3O8:H2O
Phlogopite	-2.79	41.53	44.32	KMg3AlSi3O10(OH)2
Phosgenite	-14.81	-34.62	-19.81	PbCl2:PbCO3
Plattnerite	-16.18	34.82	51.01	PbO2
Portlandite	-8.44	15.11	23.55	Ca(OH)2
Prehnite	-0.81	-12.76	-11.95	Ca2Al2Si3O10(OH)2
Pyrophyllite	1.67	-46.64	-48.31	Al2Si4O10(OH)2
Quartz	0.45	-3.67	-4.12	SiO2
Retgersite	-13.17	-15.24	-2.07	NiSO4:6H2O
Rutherfordine	-7.55	-21.97	-14.42	UO2CO3
Schoepite	-4.59	1.10	5.69	UO2(OH)2:H2O
Scorodite	-12.03	-32.27	-20.25	FeAsO4:2H2O
Se(s)	-21.84	-39.16	-17.32	Se
SeO2	-18.53	-26.91	-8.38	SeO2
Sepiolite	-0.39	15.63	16.02	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-3.03	15.63	18.66	Mg2Si3O7.5OH:3H2O
Siderite	-6.80	-17.63	-10.83	FeCO3
Siderite(d)(3)	-7.18	-17.63	-10.45	FeCO3
Silicagel	-0.55	-3.67	-3.13	SiO2
SiO2(a)	-0.88	-3.67	-2.79	SiO2
Smithsonite	-3.45	-13.35	-9.89	ZnCO3
Talc	2.77	25.28	22.52	Mg3Si4O10(OH)2
Thenardite	-8.28	-8.45	-0.17	Na2SO4
Thermonatrite	-8.86	-8.66	0.19	Na2CO3:H2O
Tremolite	8.55	67.46	58.91	Ca2Mg5Si8O22(OH)2
Trona	-13.75	-14.11	-0.36	NaHCO3:Na2CO3:2H2O
U(OH)2SO4	-36.06	-39.26	-3.20	U(OH)2SO4
U3O8(c)	-17.78	5.55	23.33	U3O8
U4O9(c)	-37.30	-38.24	-0.94	U4O9
UO2(a)	-16.50	-16.40	0.10	UO2
UO3(gamma)	-7.08	1.10	8.18	UO3
Uraninite(c)	-12.05	-16.40	-4.35	UO2
Uranophane	-7.51	9.98	17.49	Ca(UO2)2(SiO3OH)2
Wairakite	-4.20	-31.53	-27.34	CaAl2Si4O12:2H2O
Willemite	-0.35	15.78	16.14	Zn2SiO4
Witherite	-3.04	-11.63	-8.60	BaCO3
Zincite(c)	-1.94	9.73	11.67	ZnO
Zincosite	-16.60	-13.13	3.47	ZnSO4
Zn(OH)2-a	-2.72	9.73	12.45	Zn(OH)2
Zn(OH)2-b	-2.02	9.73	11.75	Zn(OH)2
Zn(OH)2-c	-2.47	9.73	12.20	Zn(OH)2
Zn(OH)2-e	-1.77	9.73	11.50	Zn(OH)2
Zn(OH)2-g	-1.98	9.73	11.71	Zn(OH)2
Zn2(OH)2SO4	-10.91	-3.41	7.50	Zn2(OH)2SO4
Zn2(OH)3Cl	-8.97	6.23	15.20	Zn2(OH)3Cl
Zn3(AsO4)2:2.5w	-19.59	-47.13	-27.55	Zn3(AsO4)2:2.5H2O
Zn3O(SO4)2	-37.05	-16.54	20.52	ZnO:2ZnSO4
Zn4(OH)6SO4	-12.35	16.05	28.40	Zn4(OH)6SO4
Zn5(OH)8Cl2	-16.31	22.19	38.50	Zn5(OH)8Cl2
ZnCl2	-24.16	-16.71	7.45	ZnCl2
ZnCO3:H2O	-3.09	-13.35	-10.26	ZnCO3:H2O
ZnMetal	-44.30	-17.65	26.64	Zn
ZnO(a)	-1.58	9.73	11.31	ZnO
ZnSiO3	2.68	6.06	3.37	ZnSiO3
ZnSO4:H2O	-12.82	-13.13	-0.31	ZnSO4:H2O

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

```
End of simulation.
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Reading input data for simulation 2.
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End of Run after 0.078 Seconds.
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```

```
   Input file: E:\Project Stuff\Models\Trace Metal_Inputst.pqi
  Output file: E:\Project Stuff\Models\Trace Metal_Inputst.pqo
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.1.2-8538\database
\wateq4f.dat

------------------
Reading data base.
------------------

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

      DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 3.1.2-8538\database
\wateq4f.dat
      TITLE Professional Project Geochemical Model
      SOLUTION   Industrial Park Well #1
              units   ppm
              pH      8.64
              temp    22.3
              O(0)            1.2
              Ca              2.35
              Mg              0.067
              Na              226
              K               1.63
              Ba              0.00295
              Cd              0
              Cu              0.00372
              Zn              0
              Pb              0.000619
              Mn              0.00652
              Se              0
              Ni              0
              Fe              0.049
              Al              0.0104
              U               0.000181
              As              0.0276
              Cl              10.4
              Alkalinity      375.5 as HCO3
              S(6)            44.1
              Si              17.6
      END
-----
TITLE
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 Professional Project Geochemical Model

-----------------------------------------
Beginning of initial solution calculations.
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Initial solution 1.     Industrial Park Well

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

      Elements           Molality       Moles

      Al                3.857e-07   3.857e-07
```

Alkalinity	6.158e-03	6.158e-03
As	3.686e-07	3.686e-07
Ba	2.149e-08	2.149e-08
Ca	5.867e-05	5.867e-05
Cl	2.935e-04	2.935e-04
Cu	5.858e-08	5.858e-08
Fe	8.780e-07	8.780e-07
K	4.171e-05	4.171e-05
Mg	2.758e-06	2.758e-06
Mn	1.188e-07	1.188e-07
Na	9.837e-03	9.837e-03
O(0)	7.505e-05	7.505e-05
Pb	2.990e-09	2.990e-09
S(6)	4.594e-04	4.594e-04
Si	2.931e-04	2.931e-04
U	7.609e-10	7.609e-10

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

pH	= 8.640
pe	= 4.000
Activity of water	= 1.000
Ionic strength	= 9.254e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 5.991e-03
Total CO2 (mol/kg)	= 5.991e-03
Temperature (°C)	= 22.30
Electrical balance (eq)	= 2.633e-03
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 15.29
Iterations	= 13
Total H	= 1.110194e+02
Total O	= 5.552726e+01

----------Redox couples----------

Redox couple	pe	Eh (volts)
O(-2)/O(0)	11.9996	0.7034

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	3.930e-06	3.551e-06	-5.406	-5.450	-0.044	(0)
H+	2.501e-09	2.291e-09	-8.602	-8.640	-0.038	0.00
H2O	5.551e+01	9.997e-01	1.744	-0.000	0.000	18.06
Al	3.857e-07					
Al(OH)4-	3.853e-07	3.491e-07	-6.414	-6.457	-0.043	(0)
Al(OH)3	4.385e-10	4.395e-10	-9.358	-9.357	0.001	(0)
Al(OH)2+	9.211e-12	8.367e-12	-11.036	-11.077	-0.042	(0)
AlOH+2	4.565e-15	3.108e-15	-14.341	-14.508	-0.167	(0)
Al+3	1.882e-18	8.556e-19	-17.725	-18.068	-0.342	(0)
AlSO4+	8.646e-19	7.835e-19	-18.063	-18.106	-0.043	(0)
Al(SO4)2-	8.100e-21	7.340e-21	-20.092	-20.134	-0.043	(0)
AlHSO4+2	2.314e-28	1.555e-28	-27.636	-27.808	-0.173	(0)
As(3)	8.761e-21					
H3AsO3	6.693e-21	6.707e-21	-20.174	-20.173	0.001	(0)
H2AsO3-	2.068e-21	1.873e-21	-20.684	-20.728	-0.043	(0)
HAsO3-2	2.158e-27	1.450e-27	-26.666	-26.839	-0.173	(0)
H4AsO3+	8.408e-30	7.613e-30	-29.075	-29.118	-0.043	(0)
AsO3-3	2.813e-34	1.151e-34	-33.551	-33.939	-0.388	(0)
As(5)	3.686e-07					
HAsO4-2	3.592e-07	2.414e-07	-6.445	-6.617	-0.173	(0)
H2AsO4-	8.933e-09	8.089e-09	-8.049	-8.092	-0.043	(0)
AsO4-3	5.394e-10	2.206e-10	-9.268	-9.656	-0.388	(0)
H3AsO4	3.594e-15	3.602e-15	-14.444	-14.443	0.001	(0)
Ba	2.149e-08					

Ba+2	1.837e-08	1.246e-08	-7.736	-7.905	-0.169	(0)
BaSO4	1.869e-09	1.873e-09	-8.728	-8.727	0.001	(0)
BaHCO3+	6.343e-10	5.743e-10	-9.198	-9.241	-0.043	(0)
BaCO3	6.163e-10	6.176e-10	-9.210	-9.209	0.001	(0)
BaOH+	2.030e-13	1.842e-13	-12.692	-12.735	-0.042	(0)
C(4)	5.991e-03					
HCO3-	5.764e-03	5.236e-03	-2.239	-2.281	-0.042	(0)
CO3-2	1.488e-04	1.013e-04	-3.827	-3.994	-0.167	(0)
CO2	2.789e-05	2.795e-05	-4.555	-4.554	0.001	(0)
NaHCO3	2.605e-05	2.610e-05	-4.584	-4.583	0.001	(0)
NaCO3-	1.605e-05	1.458e-05	-4.795	-4.836	-0.042	(0)
CaCO3	5.365e-06	5.377e-06	-5.270	-5.269	0.001	(0)
CaHCO3+	2.344e-06	2.132e-06	-5.630	-5.671	-0.041	(0)
MgCO3	1.513e-07	1.516e-07	-6.820	-6.819	0.001	(0)
MgHCO3+	1.094e-07	9.901e-08	-6.961	-7.004	-0.043	(0)
MnCO3	9.474e-08	9.494e-08	-7.023	-7.023	0.001	(0)
CuCO3	6.875e-09	6.890e-09	-8.163	-8.162	0.001	(0)
MnHCO3+	6.067e-09	5.506e-09	-8.217	-8.259	-0.042	(0)
PbCO3	2.152e-09	2.157e-09	-8.667	-8.666	0.001	(0)
Cu(CO3)2-2	1.307e-09	8.787e-10	-8.884	-9.056	-0.173	(0)
Pb(CO3)2-2	8.166e-10	5.488e-10	-9.088	-9.261	-0.173	(0)
UO2(CO3)3-4	7.197e-10	1.468e-10	-9.143	-9.833	-0.690	(0)
BaHCO3+	6.343e-10	5.743e-10	-9.198	-9.241	-0.043	(0)
BaCO3	6.163e-10	6.176e-10	-9.210	-9.209	0.001	(0)
FeCO3	1.173e-10	1.176e-10	-9.931	-9.930	0.001	(0)
UO2(CO3)2-2	4.102e-11	2.757e-11	-10.387	-10.560	-0.173	(0)
CuHCO3+	3.670e-11	3.323e-11	-10.435	-10.478	-0.043	(0)
FeHCO3+	2.798e-11	2.533e-11	-10.553	-10.596	-0.043	(0)
PbHCO3+	5.627e-12	5.095e-12	-11.250	-11.293	-0.043	(0)
UO2CO3	1.218e-14	1.220e-14	-13.915	-13.914	0.001	(0)
UO2(CO3)3-5	2.979e-26	2.486e-27	-25.526	-26.604	-1.079	(0)
(UO2)3(CO3)6-6	9.192e-28	2.572e-29	-27.037	-28.590	-1.553	(0)
U(CO3)4-4	6.061e-36	1.237e-36	-35.217	-35.908	-0.690	(0)
U(CO3)5-6	4.141e-38	1.158e-39	-37.383	-38.936	-1.553	(0)
Ca	5.867e-05					
Ca+2	4.902e-05	3.335e-05	-4.310	-4.477	-0.167	(0)
CaCO3	5.365e-06	5.377e-06	-5.270	-5.269	0.001	(0)
CaHCO3+	2.344e-06	2.132e-06	-5.630	-5.671	-0.041	(0)
CaSO4	1.942e-06	1.946e-06	-5.712	-5.711	0.001	(0)
CaOH+	2.655e-09	2.416e-09	-8.576	-8.617	-0.041	(0)
CaHSO4+	2.792e-14	2.528e-14	-13.554	-13.597	-0.043	(0)
Cl	2.935e-04					
Cl-	2.935e-04	2.654e-04	-3.532	-3.576	-0.044	(0)
MnCl+	1.406e-11	1.275e-11	-10.852	-10.894	-0.042	(0)
FeCl+	1.953e-14	1.772e-14	-13.709	-13.751	-0.042	(0)
CuCl2-	1.605e-14	1.452e-14	-13.795	-13.838	-0.043	(0)
PbCl+	1.336e-14	1.210e-14	-13.874	-13.917	-0.043	(0)
CuCl+	8.746e-15	7.915e-15	-14.058	-14.102	-0.043	(0)
MnCl2	1.474e-15	1.477e-15	-14.831	-14.830	0.001	(0)
CuCl3-2	8.912e-18	6.043e-18	-17.050	-17.219	-0.169	(0)
PbCl2	5.341e-18	5.353e-18	-17.272	-17.271	0.001	(0)
CuCl2	1.093e-18	1.095e-18	-17.961	-17.961	0.001	(0)
MnCl3-	1.190e-19	1.080e-19	-18.924	-18.967	-0.042	(0)
PbCl3-	1.225e-21	1.109e-21	-20.912	-20.955	-0.043	(0)
FeCl+2	4.314e-22	2.925e-22	-21.365	-21.534	-0.169	(0)
UO2Cl+	1.211e-23	1.096e-23	-22.917	-22.960	-0.043	(0)
CuCl3-	1.086e-24	9.825e-25	-23.964	-24.008	-0.043	(0)
FeCl2+	4.175e-25	3.780e-25	-24.379	-24.422	-0.043	(0)
PbCl4-2	2.053e-25	1.380e-25	-24.688	-24.860	-0.173	(0)
UO2Cl2	1.519e-28	1.522e-28	-27.819	-27.818	0.001	(0)
FeCl3	1.001e-29	1.003e-29	-29.000	-28.999	0.001	(0)
CuCl4-2	1.809e-30	1.227e-30	-29.742	-29.911	-0.169	(0)
UCl+3	0.000e+00	0.000e+00	-54.268	-54.656	-0.388	(0)
Cu(1)	7.351e-13					
Cu+	7.191e-13	6.479e-13	-12.143	-12.188	-0.045	(0)
CuCl2-	1.605e-14	1.452e-14	-13.795	-13.838	-0.043	(0)
CuCl3-2	8.912e-18	6.043e-18	-17.050	-17.219	-0.169	(0)
Cu(2)	5.858e-08					

Cu(OH)2	5.028e-08	5.039e-08	-7.299	-7.298	0.001	(0)
CuCO3	6.875e-09	6.890e-09	-8.163	-8.162	0.001	(0)
Cu(CO3)2-2	1.307e-09	8.787e-10	-8.884	-9.056	-0.173	(0)
CuOH+	6.107e-11	5.526e-11	-10.214	-10.258	-0.043	(0)
CuHCO3+	3.670e-11	3.323e-11	-10.435	-10.478	-0.043	(0)
Cu+2	1.848e-11	1.266e-11	-10.733	-10.897	-0.164	(0)
Cu(OH)3-	1.463e-12	1.325e-12	-11.835	-11.878	-0.043	(0)
CuSO4	7.596e-13	7.612e-13	-12.119	-12.118	0.001	(0)
CuCl+	8.746e-15	7.915e-15	-14.058	-14.102	-0.043	(0)
Cu2(OH)2+2	1.517e-15	1.020e-15	-14.819	-14.992	-0.173	(0)
Cu(OH)4-2	1.716e-16	1.154e-16	-15.765	-15.938	-0.173	(0)
CuCl2	1.093e-18	1.095e-18	-17.961	-17.961	0.001	(0)
CuCl3-	1.086e-24	9.825e-25	-23.964	-24.008	-0.043	(0)
CuCl4-2	1.809e-30	1.227e-30	-29.742	-29.911	-0.169	(0)
Fe(2)	2.244e-10					
FeCO3	1.173e-10	1.176e-10	-9.931	-9.930	0.001	(0)
Fe+2	7.062e-11	4.838e-11	-10.151	-10.315	-0.164	(0)
FeHCO3+	2.798e-11	2.533e-11	-10.553	-10.596	-0.043	(0)
FeOH+	6.003e-12	5.447e-12	-11.222	-11.264	-0.042	(0)
FeSO4	2.451e-12	2.456e-12	-11.611	-11.610	0.001	(0)
FeCl+	1.953e-14	1.772e-14	-13.709	-13.751	-0.042	(0)
Fe(OH)2	1.593e-14	1.596e-14	-13.798	-13.797	0.001	(0)
Fe(OH)3-	2.777e-16	2.520e-16	-15.556	-15.599	-0.042	(0)
FeHSO4+	4.050e-20	3.667e-20	-19.393	-19.436	-0.043	(0)
Fe(3)	8.778e-07					
Fe(OH)3	6.201e-07	6.214e-07	-6.208	-6.207	0.001	(0)
Fe(OH)4-	2.440e-07	2.217e-07	-6.613	-6.654	-0.042	(0)
Fe(OH)2+	1.370e-08	1.245e-08	-7.863	-7.905	-0.042	(0)
FeOH+2	1.409e-13	9.551e-14	-12.851	-13.020	-0.169	(0)
FeSO4+	1.358e-19	1.233e-19	-18.867	-18.909	-0.042	(0)
Fe+3	8.753e-20	3.980e-20	-19.058	-19.400	-0.342	(0)
Fe(SO4)2-	8.840e-22	8.004e-22	-21.054	-21.097	-0.043	(0)
FeCl+2	4.314e-22	2.925e-22	-21.365	-21.534	-0.169	(0)
Fe2(OH)2+4	1.347e-24	2.748e-25	-23.871	-24.561	-0.690	(0)
FeCl2+	4.175e-25	3.780e-25	-24.379	-24.422	-0.043	(0)
FeHSO4+2	1.127e-27	7.576e-28	-26.948	-27.121	-0.173	(0)
Fe3(OH)4+5	1.101e-29	9.189e-31	-28.958	-30.037	-1.079	(0)
FeCl3	1.001e-29	1.003e-29	-29.000	-28.999	0.001	(0)
H(0)	7.619e-29					
H2	3.809e-29	3.818e-29	-28.419	-28.418	0.001	(0)
K	4.171e-05					
K+	4.163e-05	3.763e-05	-4.381	-4.424	-0.044	(0)
KSO4-	8.328e-08	7.565e-08	-7.079	-7.121	-0.042	(0)
Mg	2.758e-06					
Mg+2	2.388e-06	1.635e-06	-5.622	-5.787	-0.165	(0)
MgCO3	1.513e-07	1.516e-07	-6.820	-6.819	0.001	(0)
MgHCO3+	1.094e-07	9.901e-08	-6.961	-7.004	-0.043	(0)
MgSO4	1.069e-07	1.072e-07	-6.971	-6.970	0.001	(0)
MgOH+	2.223e-09	2.025e-09	-8.653	-8.694	-0.041	(0)
Mn(2)	1.188e-07					
MnCO3	9.474e-08	9.494e-08	-7.023	-7.023	0.001	(0)
Mn+2	1.722e-08	1.180e-08	-7.764	-7.928	-0.164	(0)
MnHCO3+	6.067e-09	5.506e-09	-8.217	-8.259	-0.042	(0)
MnSO4	5.963e-10	5.976e-10	-9.225	-9.224	0.001	(0)
MnOH+	1.168e-10	1.060e-10	-9.933	-9.975	-0.042	(0)
MnCl+	1.406e-11	1.275e-11	-10.852	-10.894	-0.042	(0)
MnCl2	1.474e-15	1.477e-15	-14.831	-14.830	0.001	(0)
Mn(OH)3-	1.713e-17	1.554e-17	-16.766	-16.809	-0.042	(0)
MnCl3-	1.190e-19	1.080e-19	-18.924	-18.967	-0.042	(0)
Mn(3)	5.387e-30					
Mn+3	5.387e-30	2.449e-30	-29.269	-29.611	-0.342	(0)
Mn(6)	0.000e+00					
MnO4-2	0.000e+00	0.000e+00	-42.085	-42.254	-0.169	(0)
Mn(7)	0.000e+00					
MnO4-	0.000e+00	0.000e+00	-47.771	-47.816	-0.045	(0)
Na	9.837e-03					
Na+	9.781e-03	8.865e-03	-2.010	-2.052	-0.043	(0)
NaHCO3	2.605e-05	2.610e-05	-4.584	-4.583	0.001	(0)

NaCO3-	1.605e-05	1.458e-05	-4.795	-4.836	-0.042	(0)
NaSO4-	1.442e-05	1.310e-05	-4.841	-4.883	-0.042	(0)
O(0)	7.505e-05					
O2	3.753e-05	3.761e-05	-4.426	-4.425	0.001	(0)
Pb	2.990e-09					
PbCO3	2.152e-09	2.157e-09	-8.667	-8.666	0.001	(0)
Pb(CO3)2-2	8.166e-10	5.488e-10	-9.088	-9.261	-0.173	(0)
PbOH+	1.151e-11	1.042e-11	-10.939	-10.982	-0.043	(0)
PbHCO3+	5.627e-12	5.095e-12	-11.250	-11.293	-0.043	(0)
Pb+2	1.823e-12	1.225e-12	-11.739	-11.912	-0.173	(0)
Pb(OH)2	1.766e-12	1.770e-12	-11.753	-11.752	0.001	(0)
PbSO4	2.062e-13	2.067e-13	-12.686	-12.685	0.001	(0)
PbCl+	1.336e-14	1.210e-14	-13.874	-13.917	-0.043	(0)
Pb(OH)3-	9.793e-15	8.867e-15	-14.009	-14.052	-0.043	(0)
Pb(SO4)2-2	4.842e-16	3.254e-16	-15.315	-15.488	-0.173	(0)
Pb(OH)4-2	1.319e-17	8.865e-18	-16.880	-17.052	-0.173	(0)
PbCl2	5.341e-18	5.353e-18	-17.272	-17.271	0.001	(0)
PbCl3-	1.225e-21	1.109e-21	-20.912	-20.955	-0.043	(0)
Pb2OH+3	6.990e-22	2.859e-22	-21.156	-21.544	-0.388	(0)
PbCl4-2	2.053e-25	1.380e-25	-24.688	-24.860	-0.173	(0)
Pb3(OH)4+2	8.690e-26	5.841e-26	-25.061	-25.234	-0.173	(0)
S(6)	4.594e-04					
SO4-2	4.428e-04	3.000e-04	-3.354	-3.523	-0.169	(0)
NaSO4-	1.442e-05	1.310e-05	-4.841	-4.883	-0.042	(0)
CaSO4	1.942e-06	1.946e-06	-5.712	-5.711	0.001	(0)
MgSO4	1.069e-07	1.072e-07	-6.971	-6.970	0.001	(0)
KSO4-	8.328e-08	7.565e-08	-7.079	-7.121	-0.042	(0)
BaSO4	1.869e-09	1.873e-09	-8.728	-8.727	0.001	(0)
MnSO4	5.963e-10	5.976e-10	-9.225	-9.224	0.001	(0)
HSO4-	6.956e-11	6.304e-11	-10.158	-10.200	-0.043	(0)
FeSO4	2.451e-12	2.456e-12	-11.611	-11.610	0.001	(0)
CuSO4	7.596e-13	7.612e-13	-12.119	-12.118	0.001	(0)
PbSO4	2.062e-13	2.067e-13	-12.686	-12.685	0.001	(0)
CaHSO4+	2.792e-14	2.528e-14	-13.554	-13.597	-0.043	(0)
Pb(SO4)2-2	4.842e-16	3.254e-16	-15.315	-15.488	-0.173	(0)
AlSO4+	8.646e-19	7.835e-19	-18.063	-18.106	-0.043	(0)
FeSO4+	1.358e-19	1.233e-19	-18.867	-18.909	-0.042	(0)
FeHSO4+	4.050e-20	3.667e-20	-19.393	-19.436	-0.043	(0)
UO2SO4	1.131e-20	1.134e-20	-19.946	-19.946	0.001	(0)
Al(SO4)2-	8.100e-21	7.340e-21	-20.092	-20.134	-0.043	(0)
Fe(SO4)2-	8.840e-22	8.004e-22	-21.054	-21.097	-0.043	(0)
UO2(SO4)2-2	4.671e-23	3.139e-23	-22.331	-22.503	-0.173	(0)
FeHSO4+2	1.127e-27	7.576e-28	-26.948	-27.121	-0.173	(0)
AlHSO4+2	2.314e-28	1.555e-28	-27.636	-27.808	-0.173	(0)
U(SO4)2	0.000e+00	0.000e+00	-49.429	-49.428	0.001	(0)
USO4+2	0.000e+00	0.000e+00	-49.613	-49.786	-0.173	(0)
Si	2.931e-04					
H4SiO4	2.753e-04	2.759e-04	-3.560	-3.559	0.001	(0)
H3SiO4-	1.783e-05	1.614e-05	-4.749	-4.792	-0.043	(0)
H2SiO4-2	5.886e-10	4.008e-10	-9.230	-9.397	-0.167	(0)
U(3)	0.000e+00					
U+3	0.000e+00	0.000e+00	-65.401	-65.790	-0.388	(0)
U(4)	1.160e-27					
U(OH)4	1.160e-27	1.162e-27	-26.936	-26.935	0.001	(0)
U(OH)3+	1.111e-32	1.006e-32	-31.954	-31.997	-0.043	(0)
U(CO3)4-4	6.061e-36	1.237e-36	-35.217	-35.908	-0.690	(0)
U(CO3)5-6	4.141e-38	1.158e-39	-37.383	-38.936	-1.553	(0)
U(OH)2+2	1.711e-38	1.150e-38	-37.767	-37.939	-0.173	(0)
UOH+3	0.000e+00	0.000e+00	-44.417	-44.806	-0.388	(0)
U(SO4)2	0.000e+00	0.000e+00	-49.429	-49.428	0.001	(0)
USO4+2	0.000e+00	0.000e+00	-49.613	-49.786	-0.173	(0)
U+4	0.000e+00	0.000e+00	-52.140	-52.830	-0.690	(0)
UCl+3	0.000e+00	0.000e+00	-54.268	-54.656	-0.388	(0)
U6(OH)15+9	0.000e+00	0.000e+00	-201.089	-204.584	-3.495	(0)
U(5)	1.033e-22					
UO2+	1.033e-22	9.352e-23	-21.986	-22.029	-0.043	(0)
UO2(CO3)3-5	2.979e-26	2.486e-27	-25.526	-26.604	-1.079	(0)
U(6)	7.609e-10					

UO2(CO3)3-4	7.197e-10	1.468e-10	-9.143	-9.833	-0.690 (0)
UO2(CO3)2-2	4.102e-11	2.757e-11	-10.387	-10.560	-0.173 (0)
UO2(OH)3-	1.666e-13	1.508e-13	-12.778	-12.822	-0.043 (0)
UO2CO3	1.218e-14	1.220e-14	-13.915	-13.914	0.001 (0)
UO2OH+	7.380e-17	6.682e-17	-16.132	-16.175	-0.043 (0)
UO2(OH)4-2	1.552e-18	1.043e-18	-17.809	-17.982	-0.173 (0)
UO2+2	4.279e-20	2.876e-20	-19.369	-19.541	-0.173 (0)
UO2SO4	1.131e-20	1.134e-20	-19.946	-19.946	0.001 (0)
UO2(SO4)2-2	4.671e-23	3.139e-23	-22.331	-22.503	-0.173 (0)
UO2Cl+	1.211e-23	1.096e-23	-22.917	-22.960	-0.043 (0)
(UO2)3(CO3)6-6	9.192e-28	2.572e-29	-27.037	-28.590	-1.553 (0)
(UO2)2(OH)2+2	4.802e-28	3.227e-28	-27.319	-27.491	-0.173 (0)
UO2Cl2	1.519e-28	1.522e-28	-27.819	-27.818	0.001 (0)
(UO2)3(OH)7-	7.919e-30	7.170e-30	-29.101	-29.144	-0.043 (0)
(UO2)3(OH)5+	7.961e-32	7.208e-32	-31.099	-31.142	-0.043 (0)
(UO2)2OH+3	1.761e-33	7.203e-34	-32.754	-33.143	-0.388 (0)
(UO2)3(OH)4+2	1.616e-36	1.086e-36	-35.791	-35.964	-0.173 (0)
(UO2)4(OH)7+	2.867e-40	2.596e-40	-39.542	-39.586	-0.043 (0)

----------Saturation indices----------

Phase	SI**	log IAP	log K(295 K, 1 atm)	
Adularia	-0.78	-21.56	-20.78	KAlSi3O8
Al(OH)3(a)	-3.13	7.85	10.98	Al(OH)3
AlAsO4:2H2O	-11.89	-27.72	-15.84	AlAsO4:2H2O
Albite	-1.01	-19.19	-18.18	NaAlSi3O8
AlumK	-24.32	-29.54	-5.22	KAl(SO4)2:12H2O
Alunite	-12.77	-13.83	-1.06	KAl3(SO4)2(OH)6
Analcime	-2.80	-15.63	-12.82	NaAlSi2O6:H2O
Anglesite	-7.63	-15.43	-7.80	PbSO4
Anhydrite	-3.65	-8.00	-4.35	CaSO4
Annite	0.86	-85.20	-86.06	KFe3AlSi3O10(OH)2
Anorthite	-4.72	-24.51	-19.79	CaAl2Si2O8
Antlerite	-9.95	-1.66	8.29	Cu3(OH)4SO4
Aragonite	-0.15	-8.47	-8.32	CaCO3
Arsenolite	-38.92	-40.35	-1.43	As2O3
Artinite	-8.08	1.71	9.79	MgCO3:Mg(OH)2:3H2O
As2O5(cr)	-37.17	-28.89	8.28	As2O5
As_native	-45.38	-58.09	-12.72	As
Atacamite	-6.92	0.55	7.47	Cu2(OH)3Cl
Azurite	-6.65	-2.69	3.96	Cu3(OH)2(CO3)2
B-UO2(OH)2	-7.90	-2.26	5.64	UO2(OH)2
Ba3(AsO4)2	7.15	-43.03	-50.17	Ba3(AsO4)2
Barite	-1.41	-11.43	-10.01	BaSO4
Basaluminite	-12.10	10.60	22.70	Al4(OH)10SO4
Beidellite	-0.74	-46.42	-45.68	(NaKMg0.5)0.11Al2.33Si3.67O10(OH)2
Birnessite	-8.97	34.63	43.60	MnO2
Bixbyite	-6.87	-7.38	-0.51	Mn2O3
Boehmite	-0.92	7.85	8.77	AlOOH
Brochantite	-10.61	4.73	15.34	Cu4(OH)6SO4
Brucite	-5.53	11.49	17.02	Mg(OH)2
Ca3(AsO4)2:4w	-13.84	-32.74	-18.91	Ca3(AsO4)2:4H2O
Calcite	-0.01	-8.47	-8.47	CaCO3
Cerrusite	-2.74	-15.91	-13.16	PbCO3
Chalcanthite	-11.77	-14.42	-2.65	CuSO4:5H2O
Chalcedony	0.02	-3.56	-3.58	SiO2
Chlorite14A	-6.90	62.49	69.39	Mg5Al2Si3O10(OH)8
Chlorite7A	-10.30	62.49	72.79	Mg5Al2Si3O10(OH)8
Chrysotile	-5.18	27.36	32.54	Mg3Si2O5(OH)4
Claudetite	-38.96	-40.35	-1.39	As2O3
Clinoenstatite	-3.54	7.93	11.48	MgSiO3
CO2(g)	-3.12	-4.55	-1.44	CO2
Coffinite	-14.24	-21.83	-7.59	USiO4
Cotunnite	-14.26	-19.06	-4.81	PbCl2
Cristobalite	0.06	-3.56	-3.62	SiO2
Cu(OH)2	-2.36	6.38	8.74	Cu(OH)2
Cu2SO4	-25.98	-27.90	-1.92	Cu2SO4

Cu3(AsO4)2:6w	-16.88	-52.01	-35.12	Cu3(AsO4)2:6H2O
CuCO3	-5.26	-14.89	-9.63	CuCO3
CuMetal	-7.31	-16.19	-8.87	Cu
CuOCuSO4	-19.81	-8.04	11.77	CuO:CuSO4
CupricFerrite	13.28	19.42	6.14	CuFe2O4
Cuprite	-5.51	-7.10	-1.59	Cu2O
CuprousFerrite	11.87	2.97	-8.89	CuFeO2
CuSO4	-17.55	-14.42	3.13	CuSO4
Diaspore	0.81	7.85	7.04	AlOOH
Diopside	-2.93	17.18	20.11	CaMgSi2O6
Dioptase	-3.74	2.82	6.56	CuSiO3:H2O
Dolomite	-1.23	-18.25	-17.03	CaMg(CO3)2
Dolomite(d)	-1.79	-18.25	-16.47	CaMg(CO3)2
Epsomite	-7.15	-9.31	-2.16	MgSO4:7H2O
Fe(OH)2.7Cl.3	5.89	2.85	-3.04	Fe(OH)2.7Cl0.3
Fe(OH)3(a)	1.63	6.52	4.89	Fe(OH)3
Fe3(OH)8	-0.22	20.00	20.22	Fe3(OH)8
Forsterite	-9.20	19.43	28.63	Mg2SiO4
Gibbsite	-0.41	7.85	8.26	Al(OH)3
Goethite	7.42	6.52	-0.90	FeOOH
Greenalite	-7.03	13.78	20.81	Fe3Si2O5(OH)4
Gummite	-12.82	-2.26	10.56	UO3
Gypsum	-3.42	-8.00	-4.58	CaSO4:2H2O
H2(g)	-25.28	-28.42	-3.14	H2
H2O(g)	-1.58	-0.00	1.58	H2O
Halite	-7.20	-5.63	1.58	NaCl
Halloysite	-4.18	8.59	12.77	Al2Si2O5(OH)4
Hausmannite	-8.37	53.34	61.70	Mn3O4
Hematite	16.84	13.04	-3.80	Fe2O3
Huntite	-8.02	-37.81	-29.80	CaMg3(CO3)4
Hydrocerrusite	-8.98	-26.44	-17.46	Pb(OH)2:2PbCO3
Hydromagnesite	-19.22	-27.63	-8.41	Mg5(CO3)4(OH)2:4H2O
Illite	-1.14	-41.78	-40.63	K0.6Mg0.25Al2.3Si3.5O10(OH)2
Jarosite(ss)	-8.77	-18.60	-9.83	(K0.77Na0.03H0.2)Fe3(SO4)2(OH)6
Jarosite-K	-8.83	-17.83	-9.00	KFe3(SO4)2(OH)6
Jarosite-Na	-10.42	-15.46	-5.04	NaFe3(SO4)2(OH)6
JarositeH	-17.03	-22.05	-5.02	(H3O)Fe3(SO4)2(OH)6
Jurbanite	-9.72	-12.95	-3.23	AlOHSO4
Kaolinite	0.91	8.59	7.67	Al2Si2O5(OH)4
Kmica	3.99	17.09	13.10	KAl3Si3O10(OH)2
Langite	-12.33	4.73	17.06	Cu4(OH)6SO4:H2O
Larnakite	-9.83	-10.07	-0.24	PbO:PbSO4
Laumontite	-0.40	-31.63	-31.23	CaAl2Si4O12:4H2O
Laurionite	-7.47	-6.85	0.62	PbOHCl
Leonhardite	7.11	-63.25	-70.36	Ca2Al4Si8O24:7H2O
Litharge	-7.46	5.37	12.83	PbO
Magadiite	-4.03	-18.33	-14.30	NaSi7O13(OH)3:3H2O
Maghemite	6.65	13.04	6.39	Fe2O3
Magnesite	-1.79	-9.78	-7.99	MgCO3
Magnetite	15.93	20.00	4.08	Fe3O4
Malachite	-3.44	1.84	5.28	Cu2(OH)2CO3
Manganite	-3.35	21.99	25.34	MnOOH
Massicot	-7.65	5.37	13.02	PbO
Melanothallite	-21.86	-18.05	3.81	CuCl2
Melanterite	-11.60	-13.84	-2.24	FeSO4:7H2O
Minium	-32.99	41.38	74.38	Pb3O4
Mirabilite	-6.39	-7.63	-1.24	Na2SO4:10H2O
Mn2(SO4)3	-64.34	-69.79	-5.45	Mn2(SO4)3
Mn3(AsO4)2:8H2O	-14.39	-43.10	-28.71	Mn3(AsO4)2:8H2O
MnCl2:4H2O	-17.67	-15.08	2.59	MnCl2:4H2O
MnSO4	-14.22	-11.45	2.77	MnSO4
Montmorillonite-Aberdeen	2.74	-26.95	-29.69	(HNaK)0.14Mg0.45Fe0.33Al1.47Si3.82O10(OH)2
Montmorillonite-BelleFourche	3.09	-31.82	-34.91	(HNaK)0.09Mg0.29Fe0.24Al1.57Si3.93O10(OH)2
Montmorillonite-Ca	-0.71	-46.12	-45.42	Ca0.165Al2.33Si3.67O10(OH)2
Na4UO2(CO3)3	-23.44	-39.73	-16.29	Na4UO2(CO3)3
Nahcolite	-3.76	-4.33	-0.57	NaHCO3

Nantokite	-8.94	-15.76	-6.83	CuCl
Natron	-6.68	-8.10	-1.42	Na2CO3:10H2O
Nesquehonite	-4.20	-9.78	-5.58	MgCO3:3H2O
Nsutite	-7.93	34.63	42.56	MnO2
O2(g)	-1.55	-4.42	-2.87	O2
Pb(OH)2	-2.88	5.37	8.24	Pb(OH)2
Pb2(OH)3Cl	-10.27	-1.48	8.79	Pb2(OH)3Cl
Pb2O(OH)2	-15.46	10.74	26.20	PbO:Pb(OH)2
Pb2O3	-25.02	36.02	61.04	Pb2O3
Pb2OCO3	-10.11	-10.54	-0.42	PbO:PbCO3
Pb2SiO4	-12.76	7.18	19.93	Pb2SiO4
Pb3(AsO4)2	-19.65	-55.05	-35.40	Pb3(AsO4)2
Pb3O2CO3	-16.37	-5.17	11.20	PbCO3:2PbO
Pb3O2SO4	-15.24	-4.70	10.54	PbSO4:2PbO
Pb4(OH)6SO4	-20.43	0.67	21.10	Pb4(OH)6SO4
Pb4O3SO4	-21.67	0.67	22.33	PbSO4:3PbO
PbMetal	-24.18	-19.91	4.27	Pb
PbO:0.3H2O	-7.61	5.37	12.98	PbO:0.33H2O
PbSiO3	-5.57	1.81	7.38	PbSiO3
Phillipsite	-0.50	-20.37	-19.87	Na0.5K0.5AlSi3O8:H2O
Phlogopite	-7.71	35.87	43.58	KMg3AlSi3O10(OH)2
Phosgenite	-15.16	-34.97	-19.81	PbCl2:PbCO3
Plattnerite	-19.13	30.65	49.77	PbO2
Portlandite	-10.20	12.80	23.01	Ca(OH)2
Prehnite	-3.50	-15.26	-11.76	Ca2Al2Si3O10(OH)2
Pyrochroite	-5.85	9.35	15.20	Mn(OH)2
Pyrolusite	-7.18	34.63	41.82	MnO2
Pyrophyllite	3.88	-44.43	-48.31	Al2Si4O10(OH)2
Quartz	0.46	-3.56	-4.02	SiO2
Rhodochrosite	-0.80	-11.92	-11.12	MnCO3
Rhodochrosite(d)	-1.53	-11.92	-10.39	MnCO3
Rutherfordine	-9.10	-23.54	-14.44	UO2CO3
Schoepite	-7.75	-2.26	5.48	UO2(OH)2:H2O
Scorodite	-8.81	-29.06	-20.25	FeAsO4:2H2O
Sepiolite	-3.52	12.31	15.83	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-6.35	12.31	18.66	Mg2Si3O7.5OH:3H2O
Siderite	-3.44	-14.31	-10.87	FeCO3
Siderite(d)(3)	-3.86	-14.31	-10.45	FeCO3
Silicagel	-0.51	-3.56	-3.05	SiO2
SiO2(a)	-0.82	-3.56	-2.73	SiO2
Talc	-1.47	20.24	21.71	Mg3Si4O10(OH)2
Tenorite	-1.34	6.38	7.72	CuO
Thenardite	-7.45	-7.63	-0.18	Na2SO4
Thermonatrite	-8.24	-8.10	0.14	Na2CO3:H2O
Tremolite	-2.62	54.60	57.22	Ca2Mg5Si8O22(OH)2
Trona	-11.76	-12.43	-0.67	NaHCO3:Na2CO3:2H2O
U(OH)2SO4	-35.87	-39.07	-3.20	U(OH)2SO4
U3O8(c)	-25.56	-4.25	21.31	U3O8
U4O9(c)	-45.10	-47.80	-2.71	U4O9
UO2(a)	-18.37	-18.27	0.10	UO2
UO3(gamma)	-10.11	-2.26	7.85	UO3
Uraninite(c)	-13.60	-18.27	-4.68	UO2
Uranophane	-16.33	1.16	17.49	Ca(UO2)2(SiO3OH)2
Wairakite	-4.74	-31.63	-26.88	CaAl2Si4O12:2H2O
Witherite	-3.33	-11.90	-8.57	BaCO3

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
  For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

```
End of Run after 0.095 Seconds.
--------------------------------
```

```
   Input file: E:\Project Stuff\Models\Mixing 50_50.pqi
  Output file: E:\Project Stuff\Models\Mixing 50_50.pqo
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.2.2-10160\database
\phreeqc.dat

------------------
Reading data base.
------------------

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

      DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 3.2.2-10160\database
\phreeqc.dat
      TITLE Water Mixing Scenario Part I
      SOLUTION 1  MW-4
            units   ppm
            temp    13.9
            pH    7.87
            O(0)            7.13
            Ca              39.66
            Mg              4.05
            Na              28.4
            K               3.77
            Ba              0.07
            Be              0
            Cd              0
            Cu              0.03
            Pb              0.026
            Mn              0
            Se              0
            Ni              0.011
            Fe              0
            Al              0.05
            As              0
            Cl              14.4
            Alkalinity      132.4 as HCO3
            S(6)        32.79
            Si    12.21
      SAVE solution 1
      END
-----
TITLE
-----

 Water Mixing Scenario Part I

WARNING: Could not find element in database, As.
      Concentration is set to zero.
WARNING: Could not find element in database, Be.
      Concentration is set to zero.
WARNING: Could not find element in database, Ni.
      Concentration is set to zero.
WARNING: Could not find element in database, Se.
      Concentration is set to zero.
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------
```

Initial solution 1. MW-4

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

Elements	Molality	Moles
Al	1.854e-06	1.854e-06
Alkalinity	2.170e-03	2.170e-03
Ba	5.098e-07	5.098e-07
Ca	9.898e-04	9.898e-04
Cl	4.063e-04	4.063e-04
Cu	4.722e-07	4.722e-07
K	9.644e-05	9.644e-05
Mg	1.666e-04	1.666e-04
Na	1.236e-03	1.236e-03
O(0)	4.457e-04	4.457e-04
Pb	1.255e-07	1.255e-07
S(6)	3.414e-04	3.414e-04
Si	2.033e-04	2.033e-04

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

pH	= 7.870
pe	= 4.000
Specific Conductance (µS/cm, 13°C)	= 262
Density (g/cm³)	= 0.99948
Volume (L)	= 1.00080
Activity of water	= 1.000
Ionic strength	= 4.770e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 2.218e-03
Total CO2 (mol/kg)	= 2.218e-03
Temperature (°C)	= 13.90
Electrical balance (eq)	= 3.932e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 5.86
Iterations	= 9
Total H	= 1.110154e+02
Total O	= 5.551543e+01

----------Redox couples----------

Redox couple	pe	Eh (volts)
O(-2)/O(0)	13.6923	0.7798

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	3.297e-07	3.063e-07	-6.482	-6.514	-0.032	-4.67
H+	1.441e-08	1.349e-08	-7.841	-7.870	-0.029	0.00
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.03
Al	1.854e-06					
Al(OH)4-	1.837e-06	1.709e-06	-5.736	-5.767	-0.031	(0)
Al(OH)3	1.370e-08	1.371e-08	-7.863	-7.863	0.000	(0)
Al(OH)2+	3.254e-09	3.031e-09	-8.488	-8.518	-0.031	(0)
AlOH+2	1.953e-11	1.470e-11	-10.709	-10.833	-0.123	-27.24
Al+3	7.592e-14	4.184e-14	-13.120	-13.378	-0.259	-41.29
AlSO4+	2.836e-14	2.638e-14	-13.547	-13.579	-0.031	(0)
Al(SO4)2-	1.968e-16	1.830e-16	-15.706	-15.737	-0.031	(0)
AlHSO4+2	3.893e-23	2.909e-23	-22.410	-22.536	-0.127	(0)
Ba	5.098e-07					
Ba+2	4.639e-07	3.469e-07	-6.334	-6.460	-0.126	-13.38
BaSO4	4.021e-08	4.025e-08	-7.396	-7.395	0.000	(0)
BaHCO3+	4.968e-09	4.618e-09	-8.304	-8.336	-0.032	(0)
BaCO3	7.578e-10	7.587e-10	-9.120	-9.120	0.000	-10.82

BaOH+	9.360e-13	8.714e-13	-12.029	-12.060	-0.031	(0)
C(4)	2.218e-03					
HCO3-	2.115e-03	1.970e-03	-2.675	-2.706	-0.031	23.69
CO2	7.110e-05	7.118e-05	-4.148	-4.148	0.000	32.23
CaHCO3+	1.541e-05	1.436e-05	-4.812	-4.843	-0.030	9.19
CO3-2	7.027e-06	5.290e-06	-5.153	-5.277	-0.123	-6.47
CaCO3	5.292e-06	5.298e-06	-5.276	-5.276	0.000	-14.64
MgHCO3+	2.860e-06	2.659e-06	-5.544	-5.575	-0.032	5.12
NaHCO3	1.355e-06	1.356e-06	-5.868	-5.868	0.000	1.80
MgCO3	5.085e-07	5.091e-07	-6.294	-6.293	0.000	-17.08
PbCO3	1.174e-07	1.175e-07	-6.931	-6.930	0.000	(0)
CuCO3	9.142e-08	9.152e-08	-7.039	-7.038	0.000	(0)
NaCO3-	6.795e-08	6.318e-08	-7.168	-7.199	-0.032	-2.32
BaHCO3+	4.968e-09	4.618e-09	-8.304	-8.336	-0.032	(0)
CuHCO3+	3.421e-09	3.180e-09	-8.466	-8.498	-0.032	(0)
PbHCO3+	2.150e-09	1.999e-09	-8.667	-8.699	-0.032	(0)
Pb(CO3)2-2	2.089e-09	1.561e-09	-8.680	-8.807	-0.127	(0)
Cu(CO3)2-2	8.157e-10	6.095e-10	-9.088	-9.215	-0.127	(0)
BaCO3	7.578e-10	7.587e-10	-9.120	-9.120	0.000	-10.82
Ca	9.898e-04					
Ca+2	9.423e-04	7.090e-04	-3.026	-3.149	-0.124	-18.22
CaSO4	2.674e-05	2.677e-05	-4.573	-4.572	0.000	7.01
CaHCO3+	1.541e-05	1.436e-05	-4.812	-4.843	-0.030	9.19
CaCO3	5.292e-06	5.298e-06	-5.276	-5.276	0.000	-14.64
CaOH+	9.381e-09	8.722e-09	-8.028	-8.059	-0.032	(0)
CaHSO4+	2.210e-12	2.055e-12	-11.656	-11.687	-0.032	(0)
Cl	4.063e-04					
Cl-	4.063e-04	3.775e-04	-3.391	-3.423	-0.032	17.65
PbCl+	1.552e-11	1.443e-11	-10.809	-10.841	-0.032	7.49
CuCl2-	7.565e-12	7.032e-12	-11.121	-11.153	-0.032	(0)
CuCl+	2.002e-12	1.861e-12	-11.698	-11.730	-0.032	4.07
PbCl2	1.070e-14	1.071e-14	-13.971	-13.970	0.000	33.91
CuCl3-2	5.359e-15	4.025e-15	-14.271	-14.395	-0.124	(0)
CuCl2	3.328e-16	3.332e-16	-15.478	-15.477	0.000	15.77
PbCl3-	3.217e-18	2.991e-18	-17.493	-17.524	-0.032	64.36
PbCl4-2	6.619e-22	4.946e-22	-21.179	-21.306	-0.127	99.29
CuCl3-	3.914e-22	3.638e-22	-21.407	-21.439	-0.032	(0)
CuCl4-2	7.018e-28	5.271e-28	-27.154	-27.278	-0.124	(0)
Cu(1)	1.713e-10					
Cu+	1.637e-10	1.518e-10	-9.786	-9.819	-0.033	(0)
CuCl2-	7.565e-12	7.032e-12	-11.121	-11.153	-0.032	(0)
CuCl3-2	5.359e-15	4.025e-15	-14.271	-14.395	-0.124	(0)
Cu(2)	4.721e-07					
Cu(OH)2	3.694e-07	3.698e-07	-6.432	-6.432	0.000	(0)
CuCO3	9.142e-08	9.152e-08	-7.039	-7.038	0.000	(0)
Cu+2	4.265e-09	3.222e-09	-8.370	-8.492	-0.122	-26.44
CuHCO3+	3.421e-09	3.180e-09	-8.466	-8.498	-0.032	(0)
CuOH+	2.569e-09	2.388e-09	-8.590	-8.622	-0.032	(0)
Cu(CO3)2-2	8.157e-10	6.095e-10	-9.088	-9.215	-0.127	(0)
CuSO4	1.405e-10	1.406e-10	-9.852	-9.852	0.000	11.45
CuCl+	2.002e-12	1.861e-12	-11.698	-11.730	-0.032	4.07
Cu(OH)3-	1.777e-12	1.652e-12	-11.750	-11.782	-0.032	(0)
Cu2(OH)2+2	1.063e-12	7.943e-13	-11.973	-12.100	-0.127	(0)
CuCl2	3.328e-16	3.332e-16	-15.478	-15.477	0.000	15.77
Cu(OH)4-2	3.269e-17	2.443e-17	-16.486	-16.612	-0.127	(0)
CuCl3-	3.914e-22	3.638e-22	-21.407	-21.439	-0.032	(0)
CuCl4-2	7.018e-28	5.271e-28	-27.154	-27.278	-0.124	(0)
H(0)	2.887e-27					
H2	1.443e-27	1.445e-27	-26.841	-26.840	0.000	28.62
K	9.644e-05					
K+	9.631e-05	8.947e-05	-4.016	-4.048	-0.032	8.61
KSO4-	1.278e-07	1.190e-07	-6.894	-6.924	-0.031	33.76
Mg	1.666e-04					
Mg+2	1.584e-04	1.196e-04	-3.800	-3.922	-0.122	-21.29
MgSO4	4.817e-06	4.823e-06	-5.317	-5.317	0.000	5.34
MgHCO3+	2.860e-06	2.659e-06	-5.544	-5.575	-0.032	5.12
MgCO3	5.085e-07	5.091e-07	-6.294	-6.293	0.000	-17.08
MgOH+	1.218e-08	1.136e-08	-7.914	-7.944	-0.030	(0)

Na	1.236e-03					
Na+	1.233e-03	1.147e-03	-2.909	-2.940	-0.031	-2.12
NaHCO3	1.355e-06	1.356e-06	-5.868	-5.868	0.000	1.80
NaSO4-	1.328e-06	1.237e-06	-5.877	-5.908	-0.031	14.25
NaCO3-	6.795e-08	6.318e-08	-7.168	-7.199	-0.032	-2.32
NaOH	3.510e-20	3.514e-20	-19.455	-19.454	0.000	(0)
O(0)	4.457e-04					
O2	2.229e-04	2.231e-04	-3.652	-3.651	0.000	29.39
Pb	1.255e-07					
PbCO3	1.174e-07	1.175e-07	-6.931	-6.930	0.000	(0)
PbHCO3+	2.150e-09	1.999e-09	-8.667	-8.699	-0.032	(0)
Pb(CO3)2-2	2.089e-09	1.561e-09	-8.680	-8.807	-0.127	(0)
PbOH+	1.987e-09	1.847e-09	-8.702	-8.734	-0.032	(0)
Pb+2	1.710e-09	1.278e-09	-8.767	-8.893	-0.127	-15.34
PbSO4	1.662e-10	1.664e-10	-9.779	-9.779	0.000	(0)
Pb(OH)2	5.320e-11	5.326e-11	-10.274	-10.274	0.000	(0)
PbCl+	1.552e-11	1.443e-11	-10.809	-10.841	-0.032	7.49
Pb(SO4)2-2	2.705e-13	2.021e-13	-12.568	-12.694	-0.127	(0)
Pb(OH)3-	4.876e-14	4.533e-14	-13.312	-13.344	-0.032	(0)
PbCl2	1.070e-14	1.071e-14	-13.971	-13.970	0.000	33.91
Pb2OH+3	1.018e-16	5.284e-17	-15.992	-16.277	-0.285	(0)
Pb(OH)4-2	1.030e-17	7.697e-18	-16.987	-17.114	-0.127	(0)
PbCl3-	3.217e-18	2.991e-18	-17.493	-17.524	-0.032	64.36
Pb3(OH)4+2	1.972e-20	1.473e-20	-19.705	-19.832	-0.127	(0)
PbCl4-2	6.619e-22	4.946e-22	-21.179	-21.306	-0.127	99.29
S(6)	3.414e-04					
SO4-2	3.084e-04	2.315e-04	-3.511	-3.635	-0.125	12.78
CaSO4	2.674e-05	2.677e-05	-4.573	-4.572	0.000	7.01
MgSO4	4.817e-06	4.823e-06	-5.317	-5.317	0.000	5.34
NaSO4-	1.328e-06	1.237e-06	-5.877	-5.908	-0.031	14.25
KSO4-	1.278e-07	1.190e-07	-6.894	-6.924	-0.031	33.76
BaSO4	4.021e-08	4.025e-08	-7.396	-7.395	0.000	(0)
HSO4-	2.593e-10	2.411e-10	-9.586	-9.618	-0.032	39.37
PbSO4	1.662e-10	1.664e-10	-9.779	-9.779	0.000	(0)
CuSO4	1.405e-10	1.406e-10	-9.852	-9.852	0.000	11.45
CaHSO4+	2.210e-12	2.055e-12	-11.656	-11.687	-0.032	(0)
Pb(SO4)2-2	2.705e-13	2.021e-13	-12.568	-12.694	-0.127	(0)
AlSO4+	2.836e-14	2.638e-14	-13.547	-13.579	-0.031	(0)
Al(SO4)2-	1.968e-16	1.830e-16	-15.706	-15.737	-0.031	(0)
AlHSO4+2	3.893e-23	2.909e-23	-22.410	-22.536	-0.127	(0)
Si	2.033e-04					
H4SiO4	2.017e-04	2.019e-04	-3.695	-3.695	0.000	53.18
H3SiO4-	1.567e-06	1.457e-06	-5.805	-5.837	-0.032	27.62
H2SiO4-2	4.507e-12	3.393e-12	-11.346	-11.469	-0.123	(0)

----------Saturation indices----------

Phase	SI**	log IAP	log K(287 K, 1 atm)	
Al(OH)3(a)	-1.32	10.23	11.55	Al(OH)3
Albite	-1.06	-19.79	-18.74	NaAlSi3O8
Alunite	-4.26	-4.23	0.02	KAl3(SO4)2(OH)6
Anglesite	-4.68	-12.53	-7.85	PbSO4
Anhydrite	-2.62	-6.78	-4.16	CaSO4
Anorthite	-2.03	-22.07	-20.04	CaAl2Si2O8
Aragonite	-0.15	-8.43	-8.27	CaCO3
Barite	0.07	-10.10	-10.17	BaSO4
Ca-Montmorillonite	3.42	-43.26	-46.68	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	-0.00	-8.43	-8.43	CaCO3
Cerrusite	-0.90	-14.17	-13.27	PbCO3
Chalcedony	-0.01	-3.69	-3.69	SiO2
Chlorite(14A)	-4.21	68.47	72.67	Mg5Al2Si3O10(OH)8
Chrysotile	-5.56	28.06	33.63	Mg3Si2O5(OH)4
CO2(g)	-2.83	-4.15	-1.32	CO2
Dolomite	-0.80	-17.62	-16.82	CaMg(CO3)2
Gibbsite	1.48	10.23	8.76	Al(OH)3
Gypsum	-2.20	-6.78	-4.59	CaSO4:2H2O
H2(g)	-23.77	-26.84	-3.07	H2

```
  H2O(g)           -1.80     -0.00    1.80  H2O
  Halite           -7.92     -6.36    1.56  NaCl
  Illite            2.77    -39.05  -41.82  K0.6Mg0.25Al2.3Si3.5O10(OH)2
  K-feldspar        0.55    -20.90  -21.45  KAlSi3O8
  K-mica            9.05     23.43   14.39  KAl3Si3O10(OH)2
  Kaolinite         4.64     13.07    8.44  Al2Si2O5(OH)4
  O2(g)            -0.85     -3.65   -2.80  O2
  Pb(OH)2          -1.70      6.85    8.55  Pb(OH)2
  Quartz            0.46     -3.69   -4.15  SiO2
  Sepiolite        -3.51     12.55   16.06  Mg2Si3O7.5OH:3H2O
  Sepiolite(d)     -6.11     12.55   18.66  Mg2Si3O7.5OH:3H2O
  SiO2(a)          -0.89     -3.69   -2.81  SiO2
  Sylvite          -8.31     -7.47    0.84  KCl
  Talc             -2.04     20.67   22.71  Mg3Si4O10(OH)2
  Witherite        -3.13    -11.74   -8.60  BaCO3

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
  For ideal gases, phi = 1.

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End of simulation.
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Reading input data for simulation 2.
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      TITLE Mixing Scenario Part II
      SOLUTION 2  DI Extraction
            units   ppm
            temp    25.0
            pH    8.6
            O(0)            5.0
            Ca              3.97
            Mg              0.46
            Na              1.15
            K               0.55
            Ba              0.07
            Be              0.08
            Cd              0.007
            Cu              0.05
            Pb              0.04
            Mn              0.01
            Se              0.02
            Ni              0.01
            Fe              0.042
            Al              0.77
            As              0.04
            Cl              1.56
            Alkalinity      12.83 as HCO3
            S(6)        4.81
            Si    2.79
      END
-----
TITLE
-----

 Mixing Scenario Part II

WARNING: Could not find element in database, As.
      Concentration is set to zero.
WARNING: Could not find element in database, Be.
      Concentration is set to zero.
WARNING: Could not find element in database, Ni.
      Concentration is set to zero.
WARNING: Could not find element in database, Se.
      Concentration is set to zero.
-----------------------------------------
```

Beginning of initial solution calculations.

Initial solution 2. DI Extraction

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

Elements	Molality	Moles
Al	2.854e-05	2.854e-05
Alkalinity	2.103e-04	2.103e-04
Ba	5.097e-07	5.097e-07
Ca	9.906e-05	9.906e-05
Cd	6.228e-08	6.228e-08
Cl	4.400e-05	4.400e-05
Cu	7.869e-07	7.869e-07
Fe	7.521e-07	7.521e-07
K	1.407e-05	1.407e-05
Mg	1.892e-05	1.892e-05
Mn	1.820e-07	1.820e-07
Na	5.002e-05	5.002e-05
O(0)	3.125e-04	3.125e-04
Pb	1.931e-07	1.931e-07
S(6)	5.007e-05	5.007e-05
Si	4.644e-05	4.644e-05

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

pH	= 8.600
pe	= 4.000
Specific Conductance (µS/cm, 25°C)	= 32
Density (g/cm³)	= 0.99706
Volume (L)	= 1.00297
Activity of water	= 1.000
Ionic strength	= 4.496e-04
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 8.518e-05
Total CO2 (mol/kg)	= 8.518e-05
Temperature (°C)	= 25.00
Electrical balance (eq)	= 3.546e-05
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 6.30
Iterations	= 9
Total H	= 1.110128e+02
Total O	= 5.550729e+01

-----Redox couples-----

Redox couple	pe	Eh (volts)
O(-2)/O(0)	11.9685	0.7080

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	4.129e-06	4.029e-06	-5.384	-5.395	-0.011	-4.12
H+	2.571e-09	2.512e-09	-8.590	-8.600	-0.010	0.00
H2O	5.551e+01	1.000e+00	1.744	-0.000	0.000	18.07
Al	2.854e-05					
Al(OH)4-	2.850e-05	2.782e-05	-4.545	-4.556	-0.010	(0)
Al(OH)3	3.708e-08	3.708e-08	-7.431	-7.431	0.000	(0)
Al(OH)2+	6.475e-10	6.321e-10	-9.189	-9.199	-0.010	(0)
AlOH+2	2.230e-13	2.026e-13	-12.652	-12.693	-0.042	-27.80
Al+3	6.326e-17	5.123e-17	-16.199	-16.290	-0.092	-42.36
AlSO4+	7.410e-18	7.233e-18	-17.130	-17.141	-0.010	(0)
Al(SO4)2-	1.046e-20	1.021e-20	-19.980	-19.991	-0.010	(0)
AlHSO4+2	1.775e-27	1.611e-27	-26.751	-26.793	-0.042	(0)

Ba	5.097e-07					
Ba+2	4.989e-07	4.528e-07	-6.302	-6.344	-0.042	-12.78
BaSO4	1.013e-08	1.013e-08	-7.994	-7.994	0.000	(0)
BaHCO3+	3.584e-10	3.498e-10	-9.446	-9.456	-0.011	(0)
BaCO3	3.520e-10	3.520e-10	-9.454	-9.453	0.000	-10.70
BaOH+	6.257e-12	6.109e-12	-11.204	-11.214	-0.010	(0)
C(4)	8.518e-05					
HCO3-	8.254e-05	8.059e-05	-4.083	-4.094	-0.010	24.67
CO3-2	1.656e-06	1.505e-06	-5.781	-5.823	-0.042	-5.31
CO2	4.551e-07	4.551e-07	-6.342	-6.342	0.000	29.09
CaCO3	2.250e-07	2.251e-07	-6.648	-6.648	0.000	-14.60
PbCO3	1.379e-07	1.379e-07	-6.860	-6.860	0.000	(0)
CaHCO3+	9.377e-08	9.155e-08	-7.028	-7.038	-0.010	9.66
MgCO3	2.437e-08	2.437e-08	-7.613	-7.613	0.000	-17.09
MnCO3	1.746e-08	1.746e-08	-7.758	-7.758	0.000	(0)
MgHCO3+	1.640e-08	1.600e-08	-7.785	-7.796	-0.011	5.47
NaHCO3	2.212e-09	2.212e-09	-8.655	-8.655	0.000	1.80
CuCO3	1.912e-09	1.912e-09	-8.718	-8.718	0.000	(0)
NaCO3-	1.401e-09	1.368e-09	-8.853	-8.864	-0.011	-1.04
MnHCO3+	1.075e-09	1.049e-09	-8.969	-8.979	-0.010	(0)
Pb(CO3)2-2	5.742e-10	5.212e-10	-9.241	-9.283	-0.042	(0)
BaHCO3+	3.584e-10	3.498e-10	-9.446	-9.456	-0.011	(0)
BaCO3	3.520e-10	3.520e-10	-9.454	-9.453	0.000	-10.70
PbHCO3+	3.459e-10	3.376e-10	-9.461	-9.472	-0.011	(0)
CdHCO3+	1.404e-10	1.371e-10	-9.853	-9.863	-0.011	(0)
CdCO3	6.427e-11	6.428e-11	-10.192	-10.192	0.000	(0)
CuHCO3+	9.794e-12	9.560e-12	-11.009	-11.020	-0.011	(0)
Cu(CO3)2-2	3.991e-12	3.623e-12	-11.399	-11.441	-0.042	(0)
FeCO3	1.175e-12	1.175e-12	-11.930	-11.930	0.000	(0)
Cd(CO3)2-2	3.369e-13	3.058e-13	-12.472	-12.515	-0.042	(0)
FeHCO3+	2.688e-13	2.624e-13	-12.571	-12.581	-0.011	(0)
Ca	9.906e-05					
Ca+2	9.802e-05	8.904e-05	-4.009	-4.050	-0.042	-18.18
CaSO4	7.069e-07	7.070e-07	-6.151	-6.151	0.000	7.50
CaCO3	2.250e-07	2.251e-07	-6.648	-6.648	0.000	-14.60
CaHCO3+	9.377e-08	9.155e-08	-7.028	-7.038	-0.010	9.66
CaOH+	6.027e-09	5.883e-09	-8.220	-8.230	-0.011	(0)
CaHSO4+	1.196e-14	1.167e-14	-13.922	-13.933	-0.011	(0)
Cd	6.228e-08					
Cd+2	5.926e-08	5.378e-08	-7.227	-7.269	-0.042	-18.79
CdOH+	1.825e-09	1.781e-09	-8.739	-8.749	-0.011	(0)
CdSO4	6.925e-10	6.925e-10	-9.160	-9.160	0.000	78.05
CdCl+	2.260e-10	2.206e-10	-9.646	-9.656	-0.011	5.82
CdHCO3+	1.404e-10	1.371e-10	-9.853	-9.863	-0.011	(0)
CdCO3	6.427e-11	6.428e-11	-10.192	-10.192	0.000	(0)
Cd(OH)2	3.807e-11	3.808e-11	-10.419	-10.419	0.000	(0)
CdOHCl	3.627e-11	3.627e-11	-10.440	-10.440	0.000	(0)
Cd(SO4)2-2	3.735e-13	3.390e-13	-12.428	-12.470	-0.042	-105.68
Cd(CO3)2-2	3.369e-13	3.058e-13	-12.472	-12.515	-0.042	(0)
CdCl2	3.949e-14	3.949e-14	-13.404	-13.403	0.000	23.14
Cd(OH)3-	1.742e-15	1.701e-15	-14.759	-14.769	-0.011	(0)
Cd2OH+3	5.834e-16	4.691e-16	-15.234	-15.329	-0.095	(0)
CdCl3-	1.096e-18	1.070e-18	-17.960	-17.971	-0.011	69.31
Cd(OH)4-2	6.648e-21	6.034e-21	-20.177	-20.219	-0.042	(0)
Cl	4.400e-05					
Cl-	4.400e-05	4.295e-05	-4.357	-4.367	-0.011	18.06
CdCl+	2.260e-10	2.206e-10	-9.646	-9.656	-0.011	5.82
CdOHCl	3.627e-11	3.627e-11	-10.440	-10.440	0.000	(0)
MnCl+	2.619e-11	2.556e-11	-10.582	-10.592	-0.010	-3.10
PbCl+	9.239e-12	9.017e-12	-11.034	-11.045	-0.011	7.94
CdCl2	3.949e-14	3.949e-14	-13.404	-13.403	0.000	23.14
CuCl+	2.803e-14	2.736e-14	-13.552	-13.563	-0.011	0.62
CuCl2-	7.423e-15	7.246e-15	-14.129	-14.140	-0.011	(0)
FeCl+	1.978e-15	1.930e-15	-14.704	-14.714	-0.011	(0)
PbCl2	6.137e-16	6.138e-16	-15.212	-15.212	0.000	34.97
MnCl2	4.792e-16	4.793e-16	-15.319	-15.319	0.000	85.89
CdCl3-	1.096e-18	1.070e-18	-17.960	-17.971	-0.011	69.31
CuCl2	6.310e-19	6.311e-19	-18.200	-18.200	0.000	31.02

CuCl3-2	5.430e-19	4.932e-19	-18.265	-18.307	-0.042	(0)
PbCl3-	2.145e-20	2.094e-20	-19.669	-19.679	-0.011	65.94
MnCl3-	5.807e-21	5.669e-21	-20.236	-20.246	-0.010	43.34
FeCl+2	4.441e-23	4.033e-23	-22.353	-22.394	-0.042	(0)
PbCl4-2	4.742e-25	4.304e-25	-24.324	-24.366	-0.042	101.31
CuCl3-	9.852e-26	9.616e-26	-25.006	-25.017	-0.011	(0)
FeCl2+	7.925e-27	7.737e-27	-26.101	-26.111	-0.010	(0)
FeCl3	3.323e-32	3.323e-32	-31.479	-31.478	0.000	(0)
CuCl4-2	2.279e-32	2.070e-32	-31.642	-31.684	-0.042	(0)
Cu(1)	1.274e-11					
Cu+	1.273e-11	1.242e-11	-10.895	-10.906	-0.011	(0)
CuCl2-	7.423e-15	7.246e-15	-14.129	-14.140	-0.011	(0)
CuCl3-2	5.430e-19	4.932e-19	-18.265	-18.307	-0.042	(0)
Cu(2)	7.868e-07					
Cu(OH)2	7.837e-07	7.838e-07	-6.106	-6.106	0.000	(0)
CuCO3	1.912e-09	1.912e-09	-8.718	-8.718	0.000	(0)
CuOH+	9.654e-10	9.423e-10	-9.015	-9.026	-0.011	(0)
Cu+2	2.604e-10	2.367e-10	-9.584	-9.626	-0.042	-26.64
Cu(OH)3-	1.926e-11	1.880e-11	-10.715	-10.726	-0.011	(0)
CuHCO3+	9.794e-12	9.560e-12	-11.009	-11.020	-0.011	(0)
Cu(CO3)2-2	3.991e-12	3.623e-12	-11.399	-11.441	-0.042	(0)
CuSO4	2.157e-12	2.158e-12	-11.666	-11.666	0.000	13.09
Cu2(OH)2+2	4.281e-13	3.885e-13	-12.368	-12.411	-0.042	(0)
CuCl+	2.803e-14	2.736e-14	-13.552	-13.563	-0.011	0.62
Cu(OH)4-2	1.645e-15	1.493e-15	-14.784	-14.826	-0.042	(0)
CuCl2	6.310e-19	6.311e-19	-18.200	-18.200	0.000	31.02
CuCl3-	9.852e-26	9.616e-26	-25.006	-25.017	-0.011	(0)
CuCl4-2	2.279e-32	2.070e-32	-31.642	-31.684	-0.042	(0)
Fe(2)	4.174e-11					
Fe+2	3.583e-11	3.256e-11	-10.446	-10.487	-0.042	-22.17
FeOH+	4.199e-12	4.099e-12	-11.377	-11.387	-0.010	(0)
FeCO3	1.175e-12	1.175e-12	-11.930	-11.930	0.000	(0)
FeHCO3+	2.688e-13	2.624e-13	-12.571	-12.581	-0.011	(0)
FeSO4	2.585e-13	2.585e-13	-12.588	-12.588	0.000	18.97
Fe(OH)2	1.389e-14	1.389e-14	-13.857	-13.857	0.000	(0)
FeCl+	1.978e-15	1.930e-15	-14.704	-14.714	-0.011	(0)
Fe(OH)3-	2.104e-16	2.054e-16	-15.677	-15.687	-0.010	(0)
FeHSO4+	4.373e-21	4.268e-21	-20.359	-20.370	-0.011	(0)
Fe(3)	7.520e-07					
Fe(OH)3	5.403e-07	5.403e-07	-6.267	-6.267	0.000	(0)
Fe(OH)4-	2.010e-07	1.962e-07	-6.697	-6.707	-0.010	(0)
Fe(OH)2+	1.079e-08	1.054e-08	-7.967	-7.977	-0.010	(0)
FeOH+2	8.800e-14	7.993e-14	-13.056	-13.097	-0.042	(0)
Fe+3	3.840e-20	3.109e-20	-19.416	-19.507	-0.092	(0)
FeSO4+	1.559e-20	1.522e-20	-19.807	-19.818	-0.010	(0)
FeCl+2	4.441e-23	4.033e-23	-22.353	-22.394	-0.042	(0)
Fe(SO4)2-	1.523e-23	1.487e-23	-22.817	-22.828	-0.011	(0)
Fe2(OH)2+4	2.533e-25	1.719e-25	-24.596	-24.765	-0.168	(0)
FeCl2+	7.925e-27	7.737e-27	-26.101	-26.111	-0.010	(0)
FeHSO4+2	1.128e-28	1.024e-28	-27.948	-27.990	-0.042	(0)
Fe3(OH)4+5	6.936e-31	3.785e-31	-30.159	-30.422	-0.263	(0)
FeCl3	3.323e-32	3.323e-32	-31.479	-31.478	0.000	(0)
H(0)	8.933e-29					
H2	4.466e-29	4.467e-29	-28.350	-28.350	0.000	28.61
K	1.407e-05					
K+	1.406e-05	1.372e-05	-4.852	-4.863	-0.011	9.00
KSO4-	4.410e-09	4.305e-09	-8.356	-8.366	-0.010	34.09
Mg	1.892e-05					
Mg+2	1.868e-05	1.697e-05	-4.729	-4.770	-0.042	-21.86
MgSO4	1.776e-07	1.776e-07	-6.750	-6.750	0.000	5.84
MgOH+	2.512e-08	2.453e-08	-7.600	-7.610	-0.010	(0)
MgCO3	2.437e-08	2.437e-08	-7.613	-7.613	0.000	-17.09
MgHCO3+	1.640e-08	1.600e-08	-7.785	-7.796	-0.011	5.47
Mn(2)	1.820e-07					
Mn+2	1.608e-07	1.461e-07	-6.794	-6.835	-0.042	-21.34
MnCO3	1.746e-08	1.746e-08	-7.758	-7.758	0.000	(0)
MnOH+	1.532e-09	1.495e-09	-8.815	-8.825	-0.010	(0)
MnSO4	1.160e-09	1.160e-09	-8.936	-8.936	0.000	22.54

MnHCO3+	1.075e-09	1.049e-09	-8.969	-8.979	-0.010	(0)
MnCl+	2.619e-11	2.556e-11	-10.582	-10.592	-0.010	-3.10
MnCl2	4.792e-16	4.793e-16	-15.319	-15.319	0.000	85.89
Mn(OH)3-	1.497e-16	1.461e-16	-15.825	-15.835	-0.010	(0)
MnCl3-	5.807e-21	5.669e-21	-20.236	-20.246	-0.010	43.34
Mn(3)	5.576e-29					
Mn+3	5.576e-29	4.515e-29	-28.254	-28.345	-0.092	(0)
Na	5.002e-05					
Na+	5.001e-05	4.882e-05	-4.301	-4.311	-0.010	-1.49
NaSO4-	1.119e-08	1.092e-08	-7.951	-7.962	-0.010	13.65
NaHCO3	2.212e-09	2.212e-09	-8.655	-8.655	0.000	1.80
NaCO3-	1.401e-09	1.368e-09	-8.853	-8.864	-0.011	-1.04
NaOH	1.967e-20	1.967e-20	-19.706	-19.706	0.000	(0)
O(0)	3.125e-04					
O2	1.563e-04	1.563e-04	-3.806	-3.806	0.000	30.40
Pb	1.931e-07					
PbCO3	1.379e-07	1.379e-07	-6.860	-6.860	0.000	(0)
PbOH+	4.194e-08	4.094e-08	-7.377	-7.388	-0.011	(0)
Pb(OH)2	6.340e-09	6.341e-09	-8.198	-8.198	0.000	(0)
Pb+2	5.811e-09	5.274e-09	-8.236	-8.278	-0.042	-15.58
Pb(CO3)2-2	5.742e-10	5.212e-10	-9.241	-9.283	-0.042	(0)
PbHCO3+	3.459e-10	3.376e-10	-9.461	-9.472	-0.011	(0)
PbSO4	1.324e-10	1.324e-10	-9.878	-9.878	0.000	(0)
Pb(OH)3-	2.969e-11	2.898e-11	-10.527	-10.538	-0.011	(0)
PbCl+	9.239e-12	9.017e-12	-11.034	-11.045	-0.011	7.94
Pb(SO4)2-2	3.418e-14	3.103e-14	-13.466	-13.508	-0.042	(0)
Pb(OH)4-2	2.912e-14	2.643e-14	-13.536	-13.578	-0.042	(0)
Pb2OH+3	6.011e-15	4.834e-15	-14.221	-14.316	-0.095	(0)
Pb3(OH)4+2	5.352e-15	4.857e-15	-14.272	-14.314	-0.042	(0)
PbCl2	6.137e-16	6.138e-16	-15.212	-15.212	0.000	34.97
PbCl3-	2.145e-20	2.094e-20	-19.669	-19.679	-0.011	65.94
PbCl4-2	4.742e-25	4.304e-25	-24.324	-24.366	-0.042	101.31
S(6)	5.007e-05					
SO4-2	4.916e-05	4.465e-05	-4.308	-4.350	-0.042	14.47
CaSO4	7.069e-07	7.070e-07	-6.151	-6.151	0.000	7.50
MgSO4	1.776e-07	1.776e-07	-6.750	-6.750	0.000	5.84
NaSO4-	1.119e-08	1.092e-08	-7.951	-7.962	-0.010	13.65
BaSO4	1.013e-08	1.013e-08	-7.994	-7.994	0.000	(0)
KSO4-	4.410e-09	4.305e-09	-8.356	-8.366	-0.010	34.09
MnSO4	1.160e-09	1.160e-09	-8.936	-8.936	0.000	22.54
CdSO4	6.925e-10	6.925e-10	-9.160	-9.160	0.000	78.05
PbSO4	1.324e-10	1.324e-10	-9.878	-9.878	0.000	(0)
HSO4-	1.117e-11	1.090e-11	-10.952	-10.962	-0.011	40.27
CuSO4	2.157e-12	2.158e-12	-11.666	-11.666	0.000	13.09
Cd(SO4)2-2	3.735e-13	3.390e-13	-12.428	-12.470	-0.042	-105.68
FeSO4	2.585e-13	2.585e-13	-12.588	-12.588	0.000	18.97
Pb(SO4)2-2	3.418e-14	3.103e-14	-13.466	-13.508	-0.042	(0)
CaHSO4+	1.196e-14	1.167e-14	-13.922	-13.933	-0.011	(0)
AlSO4+	7.410e-18	7.233e-18	-17.130	-17.141	-0.010	(0)
FeSO4+	1.559e-20	1.522e-20	-19.807	-19.818	-0.010	(0)
Al(SO4)2-	1.046e-20	1.021e-20	-19.980	-19.991	-0.010	(0)
FeHSO4+	4.373e-21	4.268e-21	-20.359	-20.370	-0.011	(0)
Fe(SO4)2-	1.523e-23	1.487e-23	-22.817	-22.828	-0.011	(0)
AlHSO4+2	1.775e-27	1.611e-27	-26.751	-26.793	-0.042	(0)
FeHSO4+2	1.128e-28	1.024e-28	-27.948	-27.990	-0.042	(0)
Si	4.644e-05					
H4SiO4	4.380e-05	4.381e-05	-4.359	-4.358	0.000	52.08
H3SiO4-	2.635e-06	2.571e-06	-5.579	-5.590	-0.011	27.96
H2SiO4-2	7.665e-11	6.964e-11	-10.115	-10.157	-0.042	(0)

-------------------------------Saturation indices--------------------------------

Phase	SI**	log IAP	log K(298 K, 1 atm)	
Al(OH)3(a)	-1.29	9.51	10.80	Al(OH)3
Albite	-3.94	-21.94	-18.00	NaAlSi3O8
Alunite	-9.43	-10.83	-1.40	KAl3(SO4)2(OH)6
Anglesite	-4.84	-12.63	-7.79	PbSO4

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  Anhydrite          -4.12     -8.40   -4.28  CaSO4
  Anorthite          -2.16    -21.88  -19.71  CaAl2Si2O8
  Aragonite          -1.54     -9.87   -8.34  CaCO3
  Barite             -0.72    -10.69   -9.97  BaSO4
  Ca-Montmorillonite  0.55    -44.48  -45.03  Ca0.165Al2.33Si3.67O10(OH)2
  Calcite            -1.39     -9.87   -8.48  CaCO3
  Cd(OH)2            -3.72      9.93   13.65  Cd(OH)2
  CdSiO3             -3.49      5.57    9.06  CdSiO3
  CdSO4             -11.52    -11.62   -0.10  CdSO4
  Cerrusite          -0.97    -14.10  -13.13  PbCO3
  Chalcedony         -0.81     -4.36   -3.55  SiO2
  Chlorite(14A)      -0.29     68.09   68.38  Mg5Al2Si3O10(OH)8
  Chrysotile         -3.63     28.57   32.20  Mg3Si2O5(OH)4
  CO2(g)             -4.88     -6.34   -1.46  CO2
  Dolomite           -3.38    -20.47  -17.09  CaMg(CO3)2
  Fe(OH)3(a)          1.40      6.29    4.89  Fe(OH)3
  Gibbsite            1.40      9.51    8.11  Al(OH)3
  Goethite            7.29      6.29   -1.00  FeOOH
  Gypsum             -3.82     -8.40   -4.58  CaSO4:2H2O
  H2(g)             -25.25    -28.35   -3.10  H2
  H2O(g)             -1.50     -0.00    1.50  H2O
  Halite            -10.25     -8.68    1.57  NaCl
  Hausmannite        -4.74     56.29   61.03  Mn3O4
  Hematite           16.59     12.59   -4.01  Fe2O3
  Illite              0.10    -40.16  -40.27  K0.6Mg0.25Al2.3Si3.5O10(OH)2
  Jarosite-K        -11.27    -20.48   -9.21  KFe3(SO4)2(OH)6
  K-feldspar         -1.92    -22.49  -20.57  KAlSi3O8
  K-mica              6.49     19.19   12.70  KAl3Si3O10(OH)2
  Kaolinite           2.87     10.30    7.43  Al2Si2O5(OH)4
  Manganite          -2.38     22.96   25.34  MnOOH
  Melanterite       -12.63    -14.84   -2.21  FeSO4:7H2O
  O2(g)              -0.91     -3.81   -2.89  O2
  Otavite            -0.99    -13.09  -12.10  CdCO3
  Pb(OH)2             0.77      8.92    8.15  Pb(OH)2
  Pyrochroite        -4.84     10.36   15.20  Mn(OH)2
  Pyrolusite         -5.82     35.56   41.38  MnO2:H2O
  Quartz             -0.38     -4.36   -3.98  SiO2
  Rhodochrosite      -1.53    -12.66  -11.13  MnCO3
  Sepiolite          -3.98     11.78   15.76  Mg2Si3O7.5OH:3H2O
  Sepiolite(d)       -6.88     11.78   18.66  Mg2Si3O7.5OH:3H2O
  Siderite           -5.42    -16.31  -10.89  FeCO3
  SiO2(a)            -1.65     -4.36   -2.71  SiO2
  Sylvite           -10.13     -9.23    0.90  KCl
  Talc               -1.54     19.86   21.40  Mg3Si4O10(OH)2
  Witherite          -3.60    -12.17   -8.56  BaCO3

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
  For ideal gases, phi = 1.

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End of simulation.
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Reading input data for simulation 3.
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      TITLE Aqua Mix part III: mix 50% soln 1, 50% soln 2.
      MIX 1
              1      0.5
              2      0.5
      SAVE solution   3
      END
-----
TITLE
-----

 Aqua Mix part III: mix 50% soln 1, 50% soln 2.
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Beginning of batch-reaction calculations.
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Reaction step 1.

Using mix 1.

Mixture 1.

        5.000e-01 Solution 1  MW-4
        5.000e-01 Solution 2  DI Extraction

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

      Elements           Molality       Moles

      Al                1.520e-05   1.520e-05
      Ba                5.098e-07   5.098e-07
      C                 1.152e-03   1.152e-03
      Ca                5.444e-04   5.444e-04
      Cd                3.114e-08   3.114e-08
      Cl                2.251e-04   2.251e-04
      Cu                6.295e-07   6.295e-07
      Fe                3.760e-07   3.760e-07
      K                 5.525e-05   5.525e-05
      Mg                9.278e-05   9.278e-05
      Mn                9.101e-08   9.101e-08
      Na                6.428e-04   6.428e-04
      Pb                1.593e-07   1.593e-07
      S                 1.958e-04   1.958e-04
      Si                1.249e-04   1.249e-04

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

                                     pH  =   7.896      Charge balance
                                     pe  =  13.162      Adjusted to redox equilibrium
       Specific Conductance (µS/cm, 19°C)  = 168
                            Density (g/cm³)  =   0.99844
                                 Volume (L)  =   1.00172
                          Activity of water  =   1.000
                             Ionic strength  =   2.632e-03
                         Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   1.190e-03
                        Total CO2 (mol/kg)  =   1.152e-03
                          Temperature (°C)  =  19.45
                   Electrical balance (eq)  =   2.143e-04
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   5.86
                                Iterations  =  15
                                   Total H  = 1.110141e+02
                                   Total O  = 5.551136e+01

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

                                                 Log       Log       Log    mole V
   Species          Molality    Activity  Molality  Activity     Gamma   cm³/mol

   OH-             5.457e-07   5.158e-07    -6.263    -6.288    -0.024     -4.34
   H+              1.337e-08   1.270e-08    -7.874    -7.896    -0.023      0.00
   H2O             5.551e+01   9.999e-01     1.744    -0.000     0.000     18.05
Al            1.520e-05
   Al(OH)4-        1.508e-05   1.427e-05    -4.822    -4.846    -0.024       (0)
   Al(OH)3         1.027e-07   1.027e-07    -6.989    -6.988     0.000       (0)
   Al(OH)2+        1.429e-08   1.353e-08    -7.845    -7.869    -0.024       (0)
   AlOH+2          4.501e-11   3.616e-11   -10.347   -10.442    -0.095    -27.49
   Al+3            1.062e-13   6.661e-14   -12.974   -13.176    -0.203    -41.77
   AlSO4+          3.030e-14   2.866e-14   -13.519   -13.543    -0.024       (0)
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Al(SO4)2-	1.366e-16	1.293e-16	-15.864	-15.889	-0.024	(0)
AlHSO4+2	3.857e-23	3.085e-23	-22.414	-22.511	-0.097	(0)
Ba	5.098e-07					
Ba+2	4.777e-07	3.823e-07	-6.321	-6.418	-0.097	-13.02
BaSO4	2.804e-08	2.805e-08	-7.552	-7.552	0.000	(0)
BaHCO3+	3.407e-09	3.222e-09	-8.468	-8.492	-0.024	(0)
BaCO3	6.054e-10	6.058e-10	-9.218	-9.218	0.000	-10.75
BaOH+	1.078e-12	1.020e-12	-11.967	-11.991	-0.024	(0)
C(-4)	0.000e+00					
CH4	0.000e+00	0.000e+00	-147.802	-147.802	0.000	32.22
C(4)	1.152e-03					
HCO3-	1.106e-03	1.047e-03	-2.956	-2.980	-0.024	24.25
CO2	3.228e-05	3.230e-05	-4.491	-4.491	0.000	30.52
CaHCO3+	5.418e-06	5.132e-06	-5.266	-5.290	-0.024	9.46
CO3-2	4.268e-06	3.429e-06	-5.370	-5.465	-0.095	-5.73
CaCO3	2.202e-06	2.203e-06	-5.657	-5.657	0.000	-14.62
MgHCO3+	9.131e-07	8.634e-07	-6.039	-6.064	-0.024	5.32
NaHCO3	3.690e-07	3.692e-07	-6.433	-6.433	0.000	1.80
MgCO3	2.162e-07	2.164e-07	-6.665	-6.665	0.000	-17.08
PbCO3	1.480e-07	1.481e-07	-6.830	-6.829	0.000	(0)
CuCO3	7.689e-08	7.694e-08	-7.114	-7.114	0.000	(0)
NaCO3-	3.083e-08	2.916e-08	-7.511	-7.535	-0.024	-1.58
MnCO3	1.512e-08	1.513e-08	-7.820	-7.820	0.000	(0)
MnHCO3+	5.476e-09	5.183e-09	-8.262	-8.285	-0.024	(0)
BaHCO3+	3.407e-09	3.222e-09	-8.468	-8.492	-0.024	(0)
CuHCO3+	2.318e-09	2.192e-09	-8.635	-8.659	-0.024	(0)
PbHCO3+	2.186e-09	2.067e-09	-8.660	-8.685	-0.024	(0)
Pb(CO3)2-2	1.595e-09	1.276e-09	-8.797	-8.894	-0.097	(0)
CdHCO3+	8.044e-10	7.607e-10	-9.095	-9.119	-0.024	(0)
BaCO3	6.054e-10	6.058e-10	-9.218	-9.218	0.000	-10.75
Cu(CO3)2-2	4.153e-10	3.321e-10	-9.382	-9.479	-0.097	(0)
CdCO3	6.254e-11	6.258e-11	-10.204	-10.204	0.000	(0)
Cd(CO3)2-2	8.484e-13	6.785e-13	-12.071	-12.168	-0.097	(0)
FeHCO3+	5.644e-19	5.337e-19	-18.248	-18.273	-0.024	(0)
FeCO3	4.191e-19	4.193e-19	-18.378	-18.377	0.000	(0)
Ca	5.444e-04					
Ca+2	5.263e-04	4.226e-04	-3.279	-3.374	-0.095	-18.15
CaSO4	1.054e-05	1.055e-05	-4.977	-4.977	0.000	7.27
CaHCO3+	5.418e-06	5.132e-06	-5.266	-5.290	-0.024	9.46
CaCO3	2.202e-06	2.203e-06	-5.657	-5.657	0.000	-14.62
CaOH+	5.841e-09	5.524e-09	-8.233	-8.258	-0.024	(0)
CaHSO4+	8.628e-13	8.159e-13	-12.064	-12.088	-0.024	(0)
Cd	3.114e-08					
Cd+2	2.873e-08	2.298e-08	-7.542	-7.639	-0.097	-18.98
CdSO4	9.367e-10	9.373e-10	-9.028	-9.028	0.000	81.01
CdHCO3+	8.044e-10	7.607e-10	-9.095	-9.119	-0.024	(0)
CdCl+	4.846e-10	4.583e-10	-9.315	-9.339	-0.024	4.31
CdOH+	1.046e-10	9.896e-11	-9.980	-10.005	-0.024	(0)
CdCO3	6.254e-11	6.258e-11	-10.204	-10.204	0.000	(0)
CdOHCl	1.321e-11	1.322e-11	-10.879	-10.879	0.000	(0)
Cd(SO4)2-2	1.948e-12	1.558e-12	-11.710	-11.808	-0.097	-109.54
Cd(CO3)2-2	8.484e-13	6.785e-13	-12.071	-12.168	-0.097	(0)
Cd(OH)2	6.362e-13	6.366e-13	-12.196	-12.196	0.000	(0)
CdCl2	3.980e-13	3.983e-13	-12.400	-12.400	0.000	23.14
CdCl3-	5.194e-17	4.912e-17	-16.284	-16.309	-0.024	73.63
Cd2OH+3	1.975e-17	1.195e-17	-16.704	-16.923	-0.218	(0)
Cd(OH)3-	5.948e-18	5.625e-18	-17.226	-17.250	-0.024	(0)
Cd(OH)4-2	4.937e-24	3.948e-24	-23.307	-23.404	-0.097	(0)
CdHS+	0.000e+00	0.000e+00	-143.153	-143.177	-0.024	(0)
Cd(HS)2	0.000e+00	0.000e+00	-282.526	-282.526	0.000	(0)
Cd(HS)3-	0.000e+00	0.000e+00	-426.030	-426.055	-0.024	(0)
Cd(HS)4-2	0.000e+00	0.000e+00	-569.476	-569.573	-0.097	(0)
Cl	2.251e-04					
Cl-	2.251e-04	2.128e-04	-3.648	-3.672	-0.024	17.90
CdCl+	4.846e-10	4.583e-10	-9.315	-9.339	-0.024	4.31
MnCl+	5.089e-11	4.816e-11	-10.293	-10.317	-0.024	-4.59
PbCl+	1.936e-11	1.831e-11	-10.713	-10.737	-0.024	7.74
CdOHCl	1.321e-11	1.322e-11	-10.879	-10.879	0.000	(0)

CuCl+	1.919e-12	1.815e-12	-11.717	-11.741	-0.024	2.20
CdCl2	3.980e-13	3.983e-13	-12.400	-12.400	0.000	23.14
PbCl2	6.860e-15	6.864e-15	-14.164	-14.163	0.000	34.49
MnCl2	4.472e-15	4.475e-15	-14.349	-14.349	0.000	93.27
CuCl2	1.950e-16	1.951e-16	-15.710	-15.710	0.000	24.05
CdCl3-	5.194e-17	4.912e-17	-16.284	-16.309	-0.024	73.63
PbCl3-	1.185e-18	1.121e-18	-17.926	-17.951	-0.024	65.24
MnCl3-	2.772e-19	2.623e-19	-18.557	-18.581	-0.024	43.57
FeCl+2	3.471e-20	2.784e-20	-19.460	-19.555	-0.096	(0)
CuCl2-	2.201e-21	2.081e-21	-20.657	-20.682	-0.024	(0)
FeCl+	1.584e-21	1.498e-21	-20.800	-20.825	-0.024	(0)
CuCl3-	1.410e-22	1.333e-22	-21.851	-21.875	-0.024	(0)
PbCl4-2	1.367e-22	1.093e-22	-21.864	-21.961	-0.097	100.44
FeCl2+	3.346e-23	3.167e-23	-22.475	-22.499	-0.024	(0)
CuCl3-2	8.562e-25	6.870e-25	-24.067	-24.163	-0.096	(0)
FeCl3	6.737e-28	6.741e-28	-27.172	-27.171	0.000	(0)
CuCl4-2	1.555e-28	1.248e-28	-27.808	-27.904	-0.096	(0)
Cu(1)	1.540e-19					
Cu+	1.518e-19	1.433e-19	-18.819	-18.844	-0.025	(0)
CuCl2-	2.201e-21	2.081e-21	-20.657	-20.682	-0.024	(0)
CuCl3-2	8.562e-25	6.870e-25	-24.067	-24.163	-0.096	(0)
Cu(2)	6.295e-07					
Cu(OH)2	5.411e-07	5.414e-07	-6.267	-6.266	0.000	(0)
CuCO3	7.689e-08	7.694e-08	-7.114	-7.114	0.000	(0)
Cu+2	5.190e-09	4.178e-09	-8.285	-8.379	-0.094	-26.50
CuOH+	3.480e-09	3.291e-09	-8.458	-8.483	-0.024	(0)
CuHCO3+	2.318e-09	2.192e-09	-8.635	-8.659	-0.024	(0)
Cu(CO3)2-2	4.153e-10	3.321e-10	-9.382	-9.479	-0.097	(0)
CuSO4	1.200e-10	1.201e-10	-9.921	-9.920	0.000	12.34
Cu2(OH)2+2	3.379e-12	2.702e-12	-11.471	-11.568	-0.097	(0)
Cu(OH)3-	2.717e-12	2.569e-12	-11.566	-11.590	-0.024	(0)
CuCl+	1.919e-12	1.815e-12	-11.717	-11.741	-0.024	2.20
CuCl2	1.950e-16	1.951e-16	-15.710	-15.710	0.000	24.05
Cu(OH)4-2	5.048e-17	4.038e-17	-16.297	-16.394	-0.097	(0)
CuCl3-	1.410e-22	1.333e-22	-21.851	-21.875	-0.024	(0)
CuCl4-2	1.555e-28	1.248e-28	-27.808	-27.904	-0.096	(0)
Cu(HS)3-	0.000e+00	0.000e+00	-419.581	-419.605	-0.024	(0)
Fe(2)	7.525e-18					
Fe+2	6.333e-18	5.098e-18	-17.198	-17.293	-0.094	-22.44
FeHCO3+	5.644e-19	5.337e-19	-18.248	-18.273	-0.024	(0)
FeCO3	4.191e-19	4.193e-19	-18.378	-18.377	0.000	(0)
FeSO4	1.196e-19	1.197e-19	-18.922	-18.922	0.000	25.27
FeOH+	8.792e-20	8.321e-20	-19.056	-19.080	-0.024	(0)
FeCl+	1.584e-21	1.498e-21	-20.800	-20.825	-0.024	(0)
Fe(OH)2	3.408e-23	3.410e-23	-22.467	-22.467	0.000	(0)
Fe(OH)3-	9.974e-26	9.440e-26	-25.001	-25.025	-0.024	(0)
FeHSO4+	1.041e-26	9.842e-27	-25.983	-26.007	-0.024	(0)
Fe(HS)2	0.000e+00	0.000e+00	-299.760	-299.760	0.000	(0)
Fe(HS)3-	0.000e+00	0.000e+00	-443.407	-443.432	-0.024	(0)
Fe(3)	3.760e-07					
Fe(OH)3	3.150e-07	3.152e-07	-6.502	-6.501	0.000	(0)
Fe(OH)2+	4.199e-08	3.975e-08	-7.377	-7.401	-0.024	(0)
Fe(OH)4-	1.905e-08	1.804e-08	-7.720	-7.744	-0.024	(0)
FeOH+2	2.354e-12	1.889e-12	-11.628	-11.724	-0.096	(0)
Fe+3	8.264e-18	5.182e-18	-17.083	-17.285	-0.203	(0)
FeSO4+	7.757e-18	7.341e-18	-17.110	-17.134	-0.024	(0)
FeCl+2	3.471e-20	2.784e-20	-19.460	-19.555	-0.096	(0)
Fe(SO4)2-	2.432e-20	2.300e-20	-19.614	-19.638	-0.024	(0)
Fe2(OH)2+4	2.965e-22	1.213e-22	-21.528	-21.916	-0.388	(0)
FeCl2+	3.346e-23	3.167e-23	-22.475	-22.499	-0.024	(0)
FeHSO4+2	3.142e-25	2.513e-25	-24.503	-24.600	-0.097	(0)
Fe3(OH)4+5	6.861e-27	1.698e-27	-26.164	-26.770	-0.607	(0)
FeCl3	6.737e-28	6.741e-28	-27.172	-27.171	0.000	(0)
H(0)	0.000e+00					
H2	0.000e+00	0.000e+00	-45.242	-45.242	0.000	28.61
K	5.525e-05					
K+	5.520e-05	5.218e-05	-4.258	-4.282	-0.024	8.83
KSO4-	5.137e-08	4.864e-08	-7.289	-7.313	-0.024	33.96

Mg	9.278e-05					
Mg+2	8.950e-05	7.201e-05	-4.048	-4.143	-0.094	-21.55
MgSO4	2.135e-06	2.137e-06	-5.671	-5.670	0.000	5.61
MgHCO3+	9.131e-07	8.634e-07	-6.039	-6.064	-0.024	5.32
MgCO3	2.162e-07	2.164e-07	-6.665	-6.665	0.000	-17.08
MgOH+	1.304e-08	1.236e-08	-7.885	-7.908	-0.023	(0)
Mn(2)	9.101e-08					
Mn+2	6.900e-08	5.554e-08	-7.161	-7.255	-0.094	-20.70
MnCO3	1.512e-08	1.513e-08	-7.820	-7.820	0.000	(0)
MnHCO3+	5.476e-09	5.183e-09	-8.262	-8.285	-0.024	(0)
MnSO4	1.297e-09	1.298e-09	-8.887	-8.887	0.000	25.20
MnOH+	7.492e-11	7.091e-11	-10.125	-10.149	-0.024	(0)
MnCl+	5.089e-11	4.816e-11	-10.293	-10.317	-0.024	-4.59
MnCl2	4.472e-15	4.475e-15	-14.349	-14.349	0.000	93.27
Mn(OH)3-	4.543e-19	4.300e-19	-18.343	-18.367	-0.024	(0)
MnCl3-	2.772e-19	2.623e-19	-18.557	-18.581	-0.024	43.57
Mn(3)	1.739e-20					
Mn+3	1.739e-20	1.091e-20	-19.760	-19.962	-0.203	(0)
Na	6.428e-04					
Na+	6.420e-04	6.074e-04	-3.192	-3.217	-0.024	-1.77
NaSO4-	4.542e-07	4.300e-07	-6.343	-6.366	-0.024	14.04
NaHCO3	3.690e-07	3.692e-07	-6.433	-6.433	0.000	1.80
NaCO3-	3.083e-08	2.916e-08	-7.511	-7.535	-0.024	-1.58
NaOH	3.131e-20	3.133e-20	-19.504	-19.504	0.000	(0)
O(0)	3.791e-04					
O2	1.896e-04	1.897e-04	-3.722	-3.722	0.000	29.93
Pb	1.593e-07					
PbCO3	1.480e-07	1.481e-07	-6.830	-6.829	0.000	(0)
PbOH+	4.036e-09	3.817e-09	-8.394	-8.418	-0.024	(0)
Pb+2	3.108e-09	2.486e-09	-8.507	-8.605	-0.097	-15.43
PbHCO3+	2.186e-09	2.067e-09	-8.660	-8.685	-0.024	(0)
Pb(CO3)2-2	1.595e-09	1.276e-09	-8.797	-8.894	-0.097	(0)
PbSO4	2.045e-10	2.047e-10	-9.689	-9.689	0.000	(0)
Pb(OH)2	1.169e-10	1.170e-10	-9.932	-9.932	0.000	(0)
PbCl+	1.936e-11	1.831e-11	-10.713	-10.737	-0.024	7.74
Pb(SO4)2-2	1.966e-13	1.573e-13	-12.706	-12.803	-0.097	(0)
Pb(OH)3-	1.118e-13	1.058e-13	-12.951	-12.976	-0.024	(0)
PbCl2	6.860e-15	6.864e-15	-14.164	-14.163	0.000	34.49
Pb2OH+3	3.512e-16	2.124e-16	-15.454	-15.673	-0.218	(0)
Pb(OH)4-2	2.386e-17	1.908e-17	-16.622	-16.719	-0.097	(0)
PbCl3-	1.185e-18	1.121e-18	-17.926	-17.951	-0.024	65.24
Pb3(OH)4+2	4.170e-19	3.335e-19	-18.380	-18.477	-0.097	(0)
PbCl4-2	1.367e-22	1.093e-22	-21.864	-21.961	-0.097	100.44
Pb(HS)2	0.000e+00	0.000e+00	-284.752	-284.752	0.000	(0)
Pb(HS)3-	0.000e+00	0.000e+00	-429.136	-429.160	-0.024	(0)
S(-2)	0.000e+00					
CdHS+	0.000e+00	0.000e+00	-143.153	-143.177	-0.024	(0)
HS-	0.000e+00	0.000e+00	-145.684	-145.709	-0.024	20.33
H2S	0.000e+00	0.000e+00	-146.587	-146.587	0.000	37.14
S-2	0.000e+00	0.000e+00	-150.803	-150.899	-0.096	(0)
Cd(HS)2	0.000e+00	0.000e+00	-282.526	-282.526	0.000	(0)
Pb(HS)2	0.000e+00	0.000e+00	-284.752	-284.752	0.000	(0)
Fe(HS)2	0.000e+00	0.000e+00	-299.760	-299.760	0.000	(0)
Cu(HS)3-	0.000e+00	0.000e+00	-419.581	-419.605	-0.024	(0)
Cd(HS)3-	0.000e+00	0.000e+00	-426.030	-426.055	-0.024	(0)
Pb(HS)3-	0.000e+00	0.000e+00	-429.136	-429.160	-0.024	(0)
Fe(HS)3-	0.000e+00	0.000e+00	-443.407	-443.432	-0.024	(0)
Cd(HS)4-2	0.000e+00	0.000e+00	-569.476	-569.573	-0.097	(0)
S(6)	1.958e-04					
SO4-2	1.825e-04	1.464e-04	-3.739	-3.834	-0.096	13.78
CaSO4	1.054e-05	1.055e-05	-4.977	-4.977	0.000	7.27
MgSO4	2.135e-06	2.137e-06	-5.671	-5.670	0.000	5.61
NaSO4-	4.542e-07	4.300e-07	-6.343	-6.366	-0.024	14.04
KSO4-	5.137e-08	4.864e-08	-7.289	-7.313	-0.024	33.96
BaSO4	2.804e-08	2.805e-08	-7.552	-7.552	0.000	(0)
MnSO4	1.297e-09	1.298e-09	-8.887	-8.887	0.000	25.20
CdSO4	9.367e-10	9.373e-10	-9.028	-9.028	0.000	81.01
PbSO4	2.045e-10	2.047e-10	-9.689	-9.689	0.000	(0)

HSO4-	1.698e-10	1.606e-10	-9.770	-9.794	-0.024	39.88
CuSO4	1.200e-10	1.201e-10	-9.921	-9.920	0.000	12.34
Cd(SO4)2-2	1.948e-12	1.558e-12	-11.710	-11.808	-0.097	-109.54
CaHSO4+	8.628e-13	8.159e-13	-12.064	-12.088	-0.024	(0)
Pb(SO4)2-2	1.966e-13	1.573e-13	-12.706	-12.803	-0.097	(0)
AlSO4+	3.030e-14	2.866e-14	-13.519	-13.543	-0.024	(0)
Al(SO4)2-	1.366e-16	1.293e-16	-15.864	-15.889	-0.024	(0)
FeSO4+	7.757e-18	7.341e-18	-17.110	-17.134	-0.024	(0)
FeSO4	1.196e-19	1.197e-19	-18.922	-18.922	0.000	25.27
Fe(SO4)2-	2.432e-20	2.300e-20	-19.614	-19.638	-0.024	(0)
AlHSO4+2	3.857e-23	3.085e-23	-22.414	-22.511	-0.097	(0)
FeHSO4+2	3.142e-25	2.513e-25	-24.503	-24.600	-0.097	(0)
FeHSO4+	1.041e-26	9.842e-27	-25.983	-26.007	-0.024	(0)
Si	1.249e-04					
H4SiO4	1.236e-04	1.237e-04	-3.908	-3.908	0.000	52.58
H3SiO4-	1.243e-06	1.176e-06	-5.905	-5.930	-0.024	27.83
H2SiO4-2	5.397e-12	4.336e-12	-11.268	-11.363	-0.095	(0)

----------Saturation indices----------

Phase	SI**	log IAP	log K(292 K, 1 atm)	
Al(OH)3(a)	-0.66	10.51	11.17	Al(OH)3
Albite	-1.42	-19.79	-18.36	NaAlSi3O8
Alunite	-3.40	-4.10	-0.70	KAl3(SO4)2(OH)6
Anglesite	-4.62	-12.44	-7.82	PbSO4
Anhydrite	-2.99	-7.21	-4.22	CaSO4
Anorthite	-1.01	-20.88	-19.87	CaAl2Si2O8
Aragonite	-0.54	-8.84	-8.30	CaCO3
Barite	-0.19	-10.25	-10.06	BaSO4
Ca-Montmorillonite	3.86	-41.98	-45.84	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	-0.39	-8.84	-8.45	CaCO3
Cd(OH)2	-5.50	8.15	13.65	Cd(OH)2
CdSiO3	-5.04	4.25	9.29	CdSiO3
CdSO4	-11.58	-11.47	0.10	CdSO4
Cerrusite	-0.87	-14.07	-13.20	PbCO3
CH4(g)	-145.00	-147.80	-2.80	CH4
Chalcedony	-0.29	-3.91	-3.62	SiO2
Chlorite(14A)	-2.93	67.55	70.49	Mg5Al2Si3O10(OH)8
Chrysotile	-5.77	27.13	32.90	Mg3Si2O5(OH)4
CO2(g)	-3.10	-4.49	-1.39	CO2
Dolomite	-1.49	-18.45	-16.96	CaMg(CO3)2
Fe(OH)3(a)	1.51	6.40	4.89	Fe(OH)3
FeS(ppt)	-151.19	-155.10	-3.92	FeS
Gibbsite	2.09	10.51	8.43	Al(OH)3
Goethite	7.20	6.40	-0.80	FeOOH
Gypsum	-2.63	-7.21	-4.58	CaSO4:2H2O
H2(g)	-42.16	-45.24	-3.09	H2
H2O(g)	-1.65	-0.00	1.65	H2O
H2S(g)	-145.60	-153.60	-8.01	H2S
Halite	-8.45	-6.89	1.57	NaCl
Hausmannite	5.30	67.73	62.43	Mn3O4
Hematite	16.39	12.81	-3.58	Fe2O3
Illite	3.12	-37.90	-41.03	K0.6Mg0.25Al2.3Si3.5O10(OH)2
Jarosite-K	-7.65	-16.43	-8.78	KFe3(SO4)2(OH)6
K-feldspar	0.15	-20.85	-21.00	KAlSi3O8
K-mica	9.90	23.43	13.53	KAl3Si3O10(OH)2
Kaolinite	5.28	13.21	7.93	Al2Si2O5(OH)4
Mackinawite	-150.46	-155.10	-4.65	FeS
Manganite	4.26	29.60	25.34	MnOOH
Melanterite	-18.85	-21.13	-2.28	FeSO4:7H2O
O2(g)	-0.87	-3.72	-2.85	O2
Otavite	-1.00	-13.10	-12.10	CdCO3
Pb(OH)2	-1.16	7.19	8.34	Pb(OH)2
Pyrite	-247.96	-266.59	-18.64	FeS2
Pyrochroite	-6.66	8.54	15.20	Mn(OH)2
Pyrolusite	8.37	50.65	42.29	MnO2:H2O
Quartz	0.16	-3.91	-4.06	SiO2

```
  Rhodochrosite    -1.61    -12.72  -11.11  MnCO3
  Sepiolite        -4.33     11.58   15.91  Mg2Si3O7.5OH:3H2O
  Sepiolite(d)     -7.08     11.58   18.66  Mg2Si3O7.5OH:3H2O
  Siderite        -11.90    -22.76  -10.86  FeCO3
  SiO2(a)          -1.15     -3.91   -2.76  SiO2
  Sulfur         -109.49   -104.47    5.01  S
  Sylvite          -8.83     -7.95    0.87  KCl
  Talc             -2.72     19.32   22.04  Mg3Si4O10(OH)2
  Witherite        -3.31    -11.88   -8.58  BaCO3

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
  For ideal gases, phi = 1.

------------------
End of simulation.
------------------

-----------------------------------
Reading input data for simulation 4.
-----------------------------------

-------------------------------
End of Run after 0.254 Seconds.
-------------------------------
```

```
   Input file: E:\Project Stuff\Models\Mixing 50_50.pqi
  Output file: E:\Project Stuff\Models\Mixing 50_50.pqo
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.2.2-10160\database
\phreeqc.dat

------------------
Reading data base.
------------------

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

      DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 3.2.2-10160\database
\phreeqc.dat
      TITLE Water Mixing Scenario Part I
      SOLUTION 1  MW-4
            units   ppm
            temp    13.9
            pH    7.87
            O(0)            7.13
            Ca              39.66
            Mg              4.05
            Na              28.4
            K               3.77
            Ba              0.07
            Be              0
            Cd              0
            Cu              0.03
            Pb              0.026
            Mn              0
            Se              0
            Ni              0.011
            Fe              0
            Al              0.05
            As              0
            Cl              14.4
            Alkalinity      132.4 as HCO3
            S(6)        32.79
            Si    12.21
      SAVE solution 1
      END
-----
TITLE
-----

 Water Mixing Scenario Part I

WARNING: Could not find element in database, As.
      Concentration is set to zero.
WARNING: Could not find element in database, Be.
      Concentration is set to zero.
WARNING: Could not find element in database, Ni.
      Concentration is set to zero.
WARNING: Could not find element in database, Se.
      Concentration is set to zero.
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------
```

Initial solution 1. MW-4

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

Elements	Molality	Moles
Al	1.854e-06	1.854e-06
Alkalinity	2.170e-03	2.170e-03
Ba	5.098e-07	5.098e-07
Ca	9.898e-04	9.898e-04
Cl	4.063e-04	4.063e-04
Cu	4.722e-07	4.722e-07
K	9.644e-05	9.644e-05
Mg	1.666e-04	1.666e-04
Na	1.236e-03	1.236e-03
O(0)	4.457e-04	4.457e-04
Pb	1.255e-07	1.255e-07
S(6)	3.414e-04	3.414e-04
Si	2.033e-04	2.033e-04

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

pH	= 7.870
pe	= 4.000
Specific Conductance (µS/cm, 13°C)	= 262
Density (g/cm³)	= 0.99948
Volume (L)	= 1.00080
Activity of water	= 1.000
Ionic strength	= 4.770e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 2.218e-03
Total CO2 (mol/kg)	= 2.218e-03
Temperature (°C)	= 13.90
Electrical balance (eq)	= 3.932e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 5.86
Iterations	= 9
Total H	= 1.110154e+02
Total O	= 5.551543e+01

----------Redox couples----------

Redox couple	pe	Eh (volts)
O(-2)/O(0)	13.6923	0.7798

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	3.297e-07	3.063e-07	-6.482	-6.514	-0.032	-4.67
H+	1.441e-08	1.349e-08	-7.841	-7.870	-0.029	0.00
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.03
Al	1.854e-06					
Al(OH)4-	1.837e-06	1.709e-06	-5.736	-5.767	-0.031	(0)
Al(OH)3	1.370e-08	1.371e-08	-7.863	-7.863	0.000	(0)
Al(OH)2+	3.254e-09	3.031e-09	-8.488	-8.518	-0.031	(0)
AlOH+2	1.953e-11	1.470e-11	-10.709	-10.833	-0.123	-27.24
Al+3	7.592e-14	4.184e-14	-13.120	-13.378	-0.259	-41.29
AlSO4+	2.836e-14	2.638e-14	-13.547	-13.579	-0.031	(0)
Al(SO4)2-	1.968e-16	1.830e-16	-15.706	-15.737	-0.031	(0)
AlHSO4+2	3.893e-23	2.909e-23	-22.410	-22.536	-0.127	(0)
Ba	5.098e-07					
Ba+2	4.639e-07	3.469e-07	-6.334	-6.460	-0.126	-13.38
BaSO4	4.021e-08	4.025e-08	-7.396	-7.395	0.000	(0)
BaHCO3+	4.968e-09	4.618e-09	-8.304	-8.336	-0.032	(0)
BaCO3	7.578e-10	7.587e-10	-9.120	-9.120	0.000	-10.82

BaOH+	9.360e-13	8.714e-13	-12.029	-12.060	-0.031	(0)
C(4)	2.218e-03					
HCO3-	2.115e-03	1.970e-03	-2.675	-2.706	-0.031	23.69
CO2	7.110e-05	7.118e-05	-4.148	-4.148	0.000	32.23
CaHCO3+	1.541e-05	1.436e-05	-4.812	-4.843	-0.030	9.19
CO3-2	7.027e-06	5.290e-06	-5.153	-5.277	-0.123	-6.47
CaCO3	5.292e-06	5.298e-06	-5.276	-5.276	0.000	-14.64
MgHCO3+	2.860e-06	2.659e-06	-5.544	-5.575	-0.032	5.12
NaHCO3	1.355e-06	1.356e-06	-5.868	-5.868	0.000	1.80
MgCO3	5.085e-07	5.091e-07	-6.294	-6.293	0.000	-17.08
PbCO3	1.174e-07	1.175e-07	-6.931	-6.930	0.000	(0)
CuCO3	9.142e-08	9.152e-08	-7.039	-7.038	0.000	(0)
NaCO3-	6.795e-08	6.318e-08	-7.168	-7.199	-0.032	-2.32
BaHCO3+	4.968e-09	4.618e-09	-8.304	-8.336	-0.032	(0)
CuHCO3+	3.421e-09	3.180e-09	-8.466	-8.498	-0.032	(0)
PbHCO3+	2.150e-09	1.999e-09	-8.667	-8.699	-0.032	(0)
Pb(CO3)2-2	2.089e-09	1.561e-09	-8.680	-8.807	-0.127	(0)
Cu(CO3)2-2	8.157e-10	6.095e-10	-9.088	-9.215	-0.127	(0)
BaCO3	7.578e-10	7.587e-10	-9.120	-9.120	0.000	-10.82
Ca	9.898e-04					
Ca+2	9.423e-04	7.090e-04	-3.026	-3.149	-0.124	-18.22
CaSO4	2.674e-05	2.677e-05	-4.573	-4.572	0.000	7.01
CaHCO3+	1.541e-05	1.436e-05	-4.812	-4.843	-0.030	9.19
CaCO3	5.292e-06	5.298e-06	-5.276	-5.276	0.000	-14.64
CaOH+	9.381e-09	8.722e-09	-8.028	-8.059	-0.032	(0)
CaHSO4+	2.210e-12	2.055e-12	-11.656	-11.687	-0.032	(0)
Cl	4.063e-04					
Cl-	4.063e-04	3.775e-04	-3.391	-3.423	-0.032	17.65
PbCl+	1.552e-11	1.443e-11	-10.809	-10.841	-0.032	7.49
CuCl2-	7.565e-12	7.032e-12	-11.121	-11.153	-0.032	(0)
CuCl+	2.002e-12	1.861e-12	-11.698	-11.730	-0.032	4.07
PbCl2	1.070e-14	1.071e-14	-13.971	-13.970	0.000	33.91
CuCl3-2	5.359e-15	4.025e-15	-14.271	-14.395	-0.124	(0)
CuCl2	3.328e-16	3.332e-16	-15.478	-15.477	0.000	15.77
PbCl3-	3.217e-18	2.991e-18	-17.493	-17.524	-0.032	64.36
PbCl4-2	6.619e-22	4.946e-22	-21.179	-21.306	-0.127	99.29
CuCl3-	3.914e-22	3.638e-22	-21.407	-21.439	-0.032	(0)
CuCl4-2	7.018e-28	5.271e-28	-27.154	-27.278	-0.124	(0)
Cu(1)	1.713e-10					
Cu+	1.637e-10	1.518e-10	-9.786	-9.819	-0.033	(0)
CuCl2-	7.565e-12	7.032e-12	-11.121	-11.153	-0.032	(0)
CuCl3-2	5.359e-15	4.025e-15	-14.271	-14.395	-0.124	(0)
Cu(2)	4.721e-07					
Cu(OH)2	3.694e-07	3.698e-07	-6.432	-6.432	0.000	(0)
CuCO3	9.142e-08	9.152e-08	-7.039	-7.038	0.000	(0)
Cu+2	4.265e-09	3.222e-09	-8.370	-8.492	-0.122	-26.44
CuHCO3+	3.421e-09	3.180e-09	-8.466	-8.498	-0.032	(0)
CuOH+	2.569e-09	2.388e-09	-8.590	-8.622	-0.032	(0)
Cu(CO3)2-2	8.157e-10	6.095e-10	-9.088	-9.215	-0.127	(0)
CuSO4	1.405e-10	1.406e-10	-9.852	-9.852	0.000	11.45
CuCl+	2.002e-12	1.861e-12	-11.698	-11.730	-0.032	4.07
Cu(OH)3-	1.777e-12	1.652e-12	-11.750	-11.782	-0.032	(0)
Cu2(OH)2+2	1.063e-12	7.943e-13	-11.973	-12.100	-0.127	(0)
CuCl2	3.328e-16	3.332e-16	-15.478	-15.477	0.000	15.77
Cu(OH)4-2	3.269e-17	2.443e-17	-16.486	-16.612	-0.127	(0)
CuCl3-	3.914e-22	3.638e-22	-21.407	-21.439	-0.032	(0)
CuCl4-2	7.018e-28	5.271e-28	-27.154	-27.278	-0.124	(0)
H(0)	2.887e-27					
H2	1.443e-27	1.445e-27	-26.841	-26.840	0.000	28.62
K	9.644e-05					
K+	9.631e-05	8.947e-05	-4.016	-4.048	-0.032	8.61
KSO4-	1.278e-07	1.190e-07	-6.894	-6.924	-0.031	33.76
Mg	1.666e-04					
Mg+2	1.584e-04	1.196e-04	-3.800	-3.922	-0.122	-21.29
MgSO4	4.817e-06	4.823e-06	-5.317	-5.317	0.000	5.34
MgHCO3+	2.860e-06	2.659e-06	-5.544	-5.575	-0.032	5.12
MgCO3	5.085e-07	5.091e-07	-6.294	-6.293	0.000	-17.08
MgOH+	1.218e-08	1.136e-08	-7.914	-7.944	-0.030	(0)

Na	1.236e-03					
Na+	1.233e-03	1.147e-03	-2.909	-2.940	-0.031	-2.12
NaHCO3	1.355e-06	1.356e-06	-5.868	-5.868	0.000	1.80
NaSO4-	1.328e-06	1.237e-06	-5.877	-5.908	-0.031	14.25
NaCO3-	6.795e-08	6.318e-08	-7.168	-7.199	-0.032	-2.32
NaOH	3.510e-20	3.514e-20	-19.455	-19.454	0.000	(0)
O(0)	4.457e-04					
O2	2.229e-04	2.231e-04	-3.652	-3.651	0.000	29.39
Pb	1.255e-07					
PbCO3	1.174e-07	1.175e-07	-6.931	-6.930	0.000	(0)
PbHCO3+	2.150e-09	1.999e-09	-8.667	-8.699	-0.032	(0)
Pb(CO3)2-2	2.089e-09	1.561e-09	-8.680	-8.807	-0.127	(0)
PbOH+	1.987e-09	1.847e-09	-8.702	-8.734	-0.032	(0)
Pb+2	1.710e-09	1.278e-09	-8.767	-8.893	-0.127	-15.34
PbSO4	1.662e-10	1.664e-10	-9.779	-9.779	0.000	(0)
Pb(OH)2	5.320e-11	5.326e-11	-10.274	-10.274	0.000	(0)
PbCl+	1.552e-11	1.443e-11	-10.809	-10.841	-0.032	7.49
Pb(SO4)2-2	2.705e-13	2.021e-13	-12.568	-12.694	-0.127	(0)
Pb(OH)3-	4.876e-14	4.533e-14	-13.312	-13.344	-0.032	(0)
PbCl2	1.070e-14	1.071e-14	-13.971	-13.970	0.000	33.91
Pb2OH+3	1.018e-16	5.284e-17	-15.992	-16.277	-0.285	(0)
Pb(OH)4-2	1.030e-17	7.697e-18	-16.987	-17.114	-0.127	(0)
PbCl3-	3.217e-18	2.991e-18	-17.493	-17.524	-0.032	64.36
Pb3(OH)4+2	1.972e-20	1.473e-20	-19.705	-19.832	-0.127	(0)
PbCl4-2	6.619e-22	4.946e-22	-21.179	-21.306	-0.127	99.29
S(6)	3.414e-04					
SO4-2	3.084e-04	2.315e-04	-3.511	-3.635	-0.125	12.78
CaSO4	2.674e-05	2.677e-05	-4.573	-4.572	0.000	7.01
MgSO4	4.817e-06	4.823e-06	-5.317	-5.317	0.000	5.34
NaSO4-	1.328e-06	1.237e-06	-5.877	-5.908	-0.031	14.25
KSO4-	1.278e-07	1.190e-07	-6.894	-6.924	-0.031	33.76
BaSO4	4.021e-08	4.025e-08	-7.396	-7.395	0.000	(0)
HSO4-	2.593e-10	2.411e-10	-9.586	-9.618	-0.032	39.37
PbSO4	1.662e-10	1.664e-10	-9.779	-9.779	0.000	(0)
CuSO4	1.405e-10	1.406e-10	-9.852	-9.852	0.000	11.45
CaHSO4+	2.210e-12	2.055e-12	-11.656	-11.687	-0.032	(0)
Pb(SO4)2-2	2.705e-13	2.021e-13	-12.568	-12.694	-0.127	(0)
AlSO4+	2.836e-14	2.638e-14	-13.547	-13.579	-0.031	(0)
Al(SO4)2-	1.968e-16	1.830e-16	-15.706	-15.737	-0.031	(0)
AlHSO4+2	3.893e-23	2.909e-23	-22.410	-22.536	-0.127	(0)
Si	2.033e-04					
H4SiO4	2.017e-04	2.019e-04	-3.695	-3.695	0.000	53.18
H3SiO4-	1.567e-06	1.457e-06	-5.805	-5.837	-0.032	27.62
H2SiO4-2	4.507e-12	3.393e-12	-11.346	-11.469	-0.123	(0)

----------Saturation indices----------

Phase	SI**	log IAP	log K(287 K, 1 atm)	
Al(OH)3(a)	-1.32	10.23	11.55	Al(OH)3
Albite	-1.06	-19.79	-18.74	NaAlSi3O8
Alunite	-4.26	-4.23	0.02	KAl3(SO4)2(OH)6
Anglesite	-4.68	-12.53	-7.85	PbSO4
Anhydrite	-2.62	-6.78	-4.16	CaSO4
Anorthite	-2.03	-22.07	-20.04	CaAl2Si2O8
Aragonite	-0.15	-8.43	-8.27	CaCO3
Barite	0.07	-10.10	-10.17	BaSO4
Ca-Montmorillonite	3.42	-43.26	-46.68	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	-0.00	-8.43	-8.43	CaCO3
Cerrusite	-0.90	-14.17	-13.27	PbCO3
Chalcedony	-0.01	-3.69	-3.69	SiO2
Chlorite(14A)	-4.21	68.47	72.67	Mg5Al2Si3O10(OH)8
Chrysotile	-5.56	28.06	33.63	Mg3Si2O5(OH)4
CO2(g)	-2.83	-4.15	-1.32	CO2
Dolomite	-0.80	-17.62	-16.82	CaMg(CO3)2
Gibbsite	1.48	10.23	8.76	Al(OH)3
Gypsum	-2.20	-6.78	-4.59	CaSO4:2H2O
H2(g)	-23.77	-26.84	-3.07	H2

```
  H2O(g)           -1.80     -0.00    1.80  H2O
  Halite           -7.92     -6.36    1.56  NaCl
  Illite            2.77    -39.05  -41.82  K0.6Mg0.25Al2.3Si3.5O10(OH)2
  K-feldspar        0.55    -20.90  -21.45  KAlSi3O8
  K-mica            9.05     23.43   14.39  KAl3Si3O10(OH)2
  Kaolinite         4.64     13.07    8.44  Al2Si2O5(OH)4
  O2(g)            -0.85     -3.65   -2.80  O2
  Pb(OH)2          -1.70      6.85    8.55  Pb(OH)2
  Quartz            0.46     -3.69   -4.15  SiO2
  Sepiolite        -3.51     12.55   16.06  Mg2Si3O7.5OH:3H2O
  Sepiolite(d)     -6.11     12.55   18.66  Mg2Si3O7.5OH:3H2O
  SiO2(a)          -0.89     -3.69   -2.81  SiO2
  Sylvite          -8.31     -7.47    0.84  KCl
  Talc             -2.04     20.67   22.71  Mg3Si4O10(OH)2
  Witherite        -3.13    -11.74   -8.60  BaCO3

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
  For ideal gases, phi = 1.

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End of simulation.
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Reading input data for simulation 2.
-----------------------------------

      TITLE Mixing Scenario Part II
      SOLUTION 2  DI Extraction
            units   ppm
            temp    25.0
            pH    8.6
            O(0)            5.0
            Ca              3.97
            Mg              0.46
            Na              1.15
            K               0.55
            Ba              0.07
            Be              0.08
            Cd              0.007
            Cu              0.05
            Pb              0.04
            Mn              0.01
            Se              0.02
            Ni              0.01
            Fe              0.042
            Al              0.77
            As              0.04
            Cl              1.56
            Alkalinity      12.83 as HCO3
            S(6)        4.81
            Si    2.79
      END
-----
TITLE
-----

 Mixing Scenario Part II

WARNING: Could not find element in database, As.
      Concentration is set to zero.
WARNING: Could not find element in database, Be.
      Concentration is set to zero.
WARNING: Could not find element in database, Ni.
      Concentration is set to zero.
WARNING: Could not find element in database, Se.
      Concentration is set to zero.
-----------------------------------------
```

Beginning of initial solution calculations.

Initial solution 2. DI Extraction

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

Elements	Molality	Moles
Al	2.854e-05	2.854e-05
Alkalinity	2.103e-04	2.103e-04
Ba	5.097e-07	5.097e-07
Ca	9.906e-05	9.906e-05
Cd	6.228e-08	6.228e-08
Cl	4.400e-05	4.400e-05
Cu	7.869e-07	7.869e-07
Fe	7.521e-07	7.521e-07
K	1.407e-05	1.407e-05
Mg	1.892e-05	1.892e-05
Mn	1.820e-07	1.820e-07
Na	5.002e-05	5.002e-05
O(0)	3.125e-04	3.125e-04
Pb	1.931e-07	1.931e-07
S(6)	5.007e-05	5.007e-05
Si	4.644e-05	4.644e-05

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

pH	= 8.600
pe	= 4.000
Specific Conductance (µS/cm, 25°C)	= 32
Density (g/cm³)	= 0.99706
Volume (L)	= 1.00297
Activity of water	= 1.000
Ionic strength	= 4.496e-04
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 8.518e-05
Total CO2 (mol/kg)	= 8.518e-05
Temperature (°C)	= 25.00
Electrical balance (eq)	= 3.546e-05
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 6.30
Iterations	= 9
Total H	= 1.110128e+02
Total O	= 5.550729e+01

-----Redox couples-----

Redox couple	pe	Eh (volts)
O(-2)/O(0)	11.9685	0.7080

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	4.129e-06	4.029e-06	-5.384	-5.395	-0.011	-4.12
H+	2.571e-09	2.512e-09	-8.590	-8.600	-0.010	0.00
H2O	5.551e+01	1.000e+00	1.744	-0.000	0.000	18.07
Al	2.854e-05					
Al(OH)4-	2.850e-05	2.782e-05	-4.545	-4.556	-0.010	(0)
Al(OH)3	3.708e-08	3.708e-08	-7.431	-7.431	0.000	(0)
Al(OH)2+	6.475e-10	6.321e-10	-9.189	-9.199	-0.010	(0)
AlOH+2	2.230e-13	2.026e-13	-12.652	-12.693	-0.042	-27.80
Al+3	6.326e-17	5.123e-17	-16.199	-16.290	-0.092	-42.36
AlSO4+	7.410e-18	7.233e-18	-17.130	-17.141	-0.010	(0)
Al(SO4)2-	1.046e-20	1.021e-20	-19.980	-19.991	-0.010	(0)
AlHSO4+2	1.775e-27	1.611e-27	-26.751	-26.793	-0.042	(0)

Ba	5.097e-07					
Ba+2	4.989e-07	4.528e-07	-6.302	-6.344	-0.042	-12.78
BaSO4	1.013e-08	1.013e-08	-7.994	-7.994	0.000	(0)
BaHCO3+	3.584e-10	3.498e-10	-9.446	-9.456	-0.011	(0)
BaCO3	3.520e-10	3.520e-10	-9.454	-9.453	0.000	-10.70
BaOH+	6.257e-12	6.109e-12	-11.204	-11.214	-0.010	(0)
C(4)	8.518e-05					
HCO3-	8.254e-05	8.059e-05	-4.083	-4.094	-0.010	24.67
CO3-2	1.656e-06	1.505e-06	-5.781	-5.823	-0.042	-5.31
CO2	4.551e-07	4.551e-07	-6.342	-6.342	0.000	29.09
CaCO3	2.250e-07	2.251e-07	-6.648	-6.648	0.000	-14.60
PbCO3	1.379e-07	1.379e-07	-6.860	-6.860	0.000	(0)
CaHCO3+	9.377e-08	9.155e-08	-7.028	-7.038	-0.010	9.66
MgCO3	2.437e-08	2.437e-08	-7.613	-7.613	0.000	-17.09
MnCO3	1.746e-08	1.746e-08	-7.758	-7.758	0.000	(0)
MgHCO3+	1.640e-08	1.600e-08	-7.785	-7.796	-0.011	5.47
NaHCO3	2.212e-09	2.212e-09	-8.655	-8.655	0.000	1.80
CuCO3	1.912e-09	1.912e-09	-8.718	-8.718	0.000	(0)
NaCO3-	1.401e-09	1.368e-09	-8.853	-8.864	-0.011	-1.04
MnHCO3+	1.075e-09	1.049e-09	-8.969	-8.979	-0.010	(0)
Pb(CO3)2-2	5.742e-10	5.212e-10	-9.241	-9.283	-0.042	(0)
BaHCO3+	3.584e-10	3.498e-10	-9.446	-9.456	-0.011	(0)
BaCO3	3.520e-10	3.520e-10	-9.454	-9.453	0.000	-10.70
PbHCO3+	3.459e-10	3.376e-10	-9.461	-9.472	-0.011	(0)
CdHCO3+	1.404e-10	1.371e-10	-9.853	-9.863	-0.011	(0)
CdCO3	6.427e-11	6.428e-11	-10.192	-10.192	0.000	(0)
CuHCO3+	9.794e-12	9.560e-12	-11.009	-11.020	-0.011	(0)
Cu(CO3)2-2	3.991e-12	3.623e-12	-11.399	-11.441	-0.042	(0)
FeCO3	1.175e-12	1.175e-12	-11.930	-11.930	0.000	(0)
Cd(CO3)2-2	3.369e-13	3.058e-13	-12.472	-12.515	-0.042	(0)
FeHCO3+	2.688e-13	2.624e-13	-12.571	-12.581	-0.011	(0)
Ca	9.906e-05					
Ca+2	9.802e-05	8.904e-05	-4.009	-4.050	-0.042	-18.18
CaSO4	7.069e-07	7.070e-07	-6.151	-6.151	0.000	7.50
CaCO3	2.250e-07	2.251e-07	-6.648	-6.648	0.000	-14.60
CaHCO3+	9.377e-08	9.155e-08	-7.028	-7.038	-0.010	9.66
CaOH+	6.027e-09	5.883e-09	-8.220	-8.230	-0.011	(0)
CaHSO4+	1.196e-14	1.167e-14	-13.922	-13.933	-0.011	(0)
Cd	6.228e-08					
Cd+2	5.926e-08	5.378e-08	-7.227	-7.269	-0.042	-18.79
CdOH+	1.825e-09	1.781e-09	-8.739	-8.749	-0.011	(0)
CdSO4	6.925e-10	6.925e-10	-9.160	-9.160	0.000	78.05
CdCl+	2.260e-10	2.206e-10	-9.646	-9.656	-0.011	5.82
CdHCO3+	1.404e-10	1.371e-10	-9.853	-9.863	-0.011	(0)
CdCO3	6.427e-11	6.428e-11	-10.192	-10.192	0.000	(0)
Cd(OH)2	3.807e-11	3.808e-11	-10.419	-10.419	0.000	(0)
CdOHCl	3.627e-11	3.627e-11	-10.440	-10.440	0.000	(0)
Cd(SO4)2-2	3.735e-13	3.390e-13	-12.428	-12.470	-0.042	-105.68
Cd(CO3)2-2	3.369e-13	3.058e-13	-12.472	-12.515	-0.042	(0)
CdCl2	3.949e-14	3.949e-14	-13.404	-13.403	0.000	23.14
Cd(OH)3-	1.742e-15	1.701e-15	-14.759	-14.769	-0.011	(0)
Cd2OH+3	5.834e-16	4.691e-16	-15.234	-15.329	-0.095	(0)
CdCl3-	1.096e-18	1.070e-18	-17.960	-17.971	-0.011	69.31
Cd(OH)4-2	6.648e-21	6.034e-21	-20.177	-20.219	-0.042	(0)
Cl	4.400e-05					
Cl-	4.400e-05	4.295e-05	-4.357	-4.367	-0.011	18.06
CdCl+	2.260e-10	2.206e-10	-9.646	-9.656	-0.011	5.82
CdOHCl	3.627e-11	3.627e-11	-10.440	-10.440	0.000	(0)
MnCl+	2.619e-11	2.556e-11	-10.582	-10.592	-0.010	-3.10
PbCl+	9.239e-12	9.017e-12	-11.034	-11.045	-0.011	7.94
CdCl2	3.949e-14	3.949e-14	-13.404	-13.403	0.000	23.14
CuCl+	2.803e-14	2.736e-14	-13.552	-13.563	-0.011	0.62
CuCl2-	7.423e-15	7.246e-15	-14.129	-14.140	-0.011	(0)
FeCl+	1.978e-15	1.930e-15	-14.704	-14.714	-0.011	(0)
PbCl2	6.137e-16	6.138e-16	-15.212	-15.212	0.000	34.97
MnCl2	4.792e-16	4.793e-16	-15.319	-15.319	0.000	85.89
CdCl3-	1.096e-18	1.070e-18	-17.960	-17.971	-0.011	69.31
CuCl2	6.310e-19	6.311e-19	-18.200	-18.200	0.000	31.02

CuCl3-2	5.430e-19	4.932e-19	-18.265	-18.307	-0.042	(0)
PbCl3-	2.145e-20	2.094e-20	-19.669	-19.679	-0.011	65.94
MnCl3-	5.807e-21	5.669e-21	-20.236	-20.246	-0.010	43.34
FeCl+2	4.441e-23	4.033e-23	-22.353	-22.394	-0.042	(0)
PbCl4-2	4.742e-25	4.304e-25	-24.324	-24.366	-0.042	101.31
CuCl3-	9.852e-26	9.616e-26	-25.006	-25.017	-0.011	(0)
FeCl2+	7.925e-27	7.737e-27	-26.101	-26.111	-0.010	(0)
FeCl3	3.323e-32	3.323e-32	-31.479	-31.478	0.000	(0)
CuCl4-2	2.279e-32	2.070e-32	-31.642	-31.684	-0.042	(0)
Cu(1)	1.274e-11					
Cu+	1.273e-11	1.242e-11	-10.895	-10.906	-0.011	(0)
CuCl2-	7.423e-15	7.246e-15	-14.129	-14.140	-0.011	(0)
CuCl3-2	5.430e-19	4.932e-19	-18.265	-18.307	-0.042	(0)
Cu(2)	7.868e-07					
Cu(OH)2	7.837e-07	7.838e-07	-6.106	-6.106	0.000	(0)
CuCO3	1.912e-09	1.912e-09	-8.718	-8.718	0.000	(0)
CuOH+	9.654e-10	9.423e-10	-9.015	-9.026	-0.011	(0)
Cu+2	2.604e-10	2.367e-10	-9.584	-9.626	-0.042	-26.64
Cu(OH)3-	1.926e-11	1.880e-11	-10.715	-10.726	-0.011	(0)
CuHCO3+	9.794e-12	9.560e-12	-11.009	-11.020	-0.011	(0)
Cu(CO3)2-2	3.991e-12	3.623e-12	-11.399	-11.441	-0.042	(0)
CuSO4	2.157e-12	2.158e-12	-11.666	-11.666	0.000	13.09
Cu2(OH)2+2	4.281e-13	3.885e-13	-12.368	-12.411	-0.042	(0)
CuCl+	2.803e-14	2.736e-14	-13.552	-13.563	-0.011	0.62
Cu(OH)4-2	1.645e-15	1.493e-15	-14.784	-14.826	-0.042	(0)
CuCl2	6.310e-19	6.311e-19	-18.200	-18.200	0.000	31.02
CuCl3-	9.852e-26	9.616e-26	-25.006	-25.017	-0.011	(0)
CuCl4-2	2.279e-32	2.070e-32	-31.642	-31.684	-0.042	(0)
Fe(2)	4.174e-11					
Fe+2	3.583e-11	3.256e-11	-10.446	-10.487	-0.042	-22.17
FeOH+	4.199e-12	4.099e-12	-11.377	-11.387	-0.010	(0)
FeCO3	1.175e-12	1.175e-12	-11.930	-11.930	0.000	(0)
FeHCO3+	2.688e-13	2.624e-13	-12.571	-12.581	-0.011	(0)
FeSO4	2.585e-13	2.585e-13	-12.588	-12.588	0.000	18.97
Fe(OH)2	1.389e-14	1.389e-14	-13.857	-13.857	0.000	(0)
FeCl+	1.978e-15	1.930e-15	-14.704	-14.714	-0.011	(0)
Fe(OH)3-	2.104e-16	2.054e-16	-15.677	-15.687	-0.010	(0)
FeHSO4+	4.373e-21	4.268e-21	-20.359	-20.370	-0.011	(0)
Fe(3)	7.520e-07					
Fe(OH)3	5.403e-07	5.403e-07	-6.267	-6.267	0.000	(0)
Fe(OH)4-	2.010e-07	1.962e-07	-6.697	-6.707	-0.010	(0)
Fe(OH)2+	1.079e-08	1.054e-08	-7.967	-7.977	-0.010	(0)
FeOH+2	8.800e-14	7.993e-14	-13.056	-13.097	-0.042	(0)
Fe+3	3.840e-20	3.109e-20	-19.416	-19.507	-0.092	(0)
FeSO4+	1.559e-20	1.522e-20	-19.807	-19.818	-0.010	(0)
FeCl+2	4.441e-23	4.033e-23	-22.353	-22.394	-0.042	(0)
Fe(SO4)2-	1.523e-23	1.487e-23	-22.817	-22.828	-0.011	(0)
Fe2(OH)2+4	2.533e-25	1.719e-25	-24.596	-24.765	-0.168	(0)
FeCl2+	7.925e-27	7.737e-27	-26.101	-26.111	-0.010	(0)
FeHSO4+2	1.128e-28	1.024e-28	-27.948	-27.990	-0.042	(0)
Fe3(OH)4+5	6.936e-31	3.785e-31	-30.159	-30.422	-0.263	(0)
FeCl3	3.323e-32	3.323e-32	-31.479	-31.478	0.000	(0)
H(0)	8.933e-29					
H2	4.466e-29	4.467e-29	-28.350	-28.350	0.000	28.61
K	1.407e-05					
K+	1.406e-05	1.372e-05	-4.852	-4.863	-0.011	9.00
KSO4-	4.410e-09	4.305e-09	-8.356	-8.366	-0.010	34.09
Mg	1.892e-05					
Mg+2	1.868e-05	1.697e-05	-4.729	-4.770	-0.042	-21.86
MgSO4	1.776e-07	1.776e-07	-6.750	-6.750	0.000	5.84
MgOH+	2.512e-08	2.453e-08	-7.600	-7.610	-0.010	(0)
MgCO3	2.437e-08	2.437e-08	-7.613	-7.613	0.000	-17.09
MgHCO3+	1.640e-08	1.600e-08	-7.785	-7.796	-0.011	5.47
Mn(2)	1.820e-07					
Mn+2	1.608e-07	1.461e-07	-6.794	-6.835	-0.042	-21.34
MnCO3	1.746e-08	1.746e-08	-7.758	-7.758	0.000	(0)
MnOH+	1.532e-09	1.495e-09	-8.815	-8.825	-0.010	(0)
MnSO4	1.160e-09	1.160e-09	-8.936	-8.936	0.000	22.54

MnHCO3+	1.075e-09	1.049e-09	-8.969	-8.979	-0.010	(0)
MnCl+	2.619e-11	2.556e-11	-10.582	-10.592	-0.010	-3.10
MnCl2	4.792e-16	4.793e-16	-15.319	-15.319	0.000	85.89
Mn(OH)3-	1.497e-16	1.461e-16	-15.825	-15.835	-0.010	(0)
MnCl3-	5.807e-21	5.669e-21	-20.236	-20.246	-0.010	43.34
Mn(3)	5.576e-29					
Mn+3	5.576e-29	4.515e-29	-28.254	-28.345	-0.092	(0)
Na	5.002e-05					
Na+	5.001e-05	4.882e-05	-4.301	-4.311	-0.010	-1.49
NaSO4-	1.119e-08	1.092e-08	-7.951	-7.962	-0.010	13.65
NaHCO3	2.212e-09	2.212e-09	-8.655	-8.655	0.000	1.80
NaCO3-	1.401e-09	1.368e-09	-8.853	-8.864	-0.011	-1.04
NaOH	1.967e-20	1.967e-20	-19.706	-19.706	0.000	(0)
O(0)	3.125e-04					
O2	1.563e-04	1.563e-04	-3.806	-3.806	0.000	30.40
Pb	1.931e-07					
PbCO3	1.379e-07	1.379e-07	-6.860	-6.860	0.000	(0)
PbOH+	4.194e-08	4.094e-08	-7.377	-7.388	-0.011	(0)
Pb(OH)2	6.340e-09	6.341e-09	-8.198	-8.198	0.000	(0)
Pb+2	5.811e-09	5.274e-09	-8.236	-8.278	-0.042	-15.58
Pb(CO3)2-2	5.742e-10	5.212e-10	-9.241	-9.283	-0.042	(0)
PbHCO3+	3.459e-10	3.376e-10	-9.461	-9.472	-0.011	(0)
PbSO4	1.324e-10	1.324e-10	-9.878	-9.878	0.000	(0)
Pb(OH)3-	2.969e-11	2.898e-11	-10.527	-10.538	-0.011	(0)
PbCl+	9.239e-12	9.017e-12	-11.034	-11.045	-0.011	7.94
Pb(SO4)2-2	3.418e-14	3.103e-14	-13.466	-13.508	-0.042	(0)
Pb(OH)4-2	2.912e-14	2.643e-14	-13.536	-13.578	-0.042	(0)
Pb2OH+3	6.011e-15	4.834e-15	-14.221	-14.316	-0.095	(0)
Pb3(OH)4+2	5.352e-15	4.857e-15	-14.272	-14.314	-0.042	(0)
PbCl2	6.137e-16	6.138e-16	-15.212	-15.212	0.000	34.97
PbCl3-	2.145e-20	2.094e-20	-19.669	-19.679	-0.011	65.94
PbCl4-2	4.742e-25	4.304e-25	-24.324	-24.366	-0.042	101.31
S(6)	5.007e-05					
SO4-2	4.916e-05	4.465e-05	-4.308	-4.350	-0.042	14.47
CaSO4	7.069e-07	7.070e-07	-6.151	-6.151	0.000	7.50
MgSO4	1.776e-07	1.776e-07	-6.750	-6.750	0.000	5.84
NaSO4-	1.119e-08	1.092e-08	-7.951	-7.962	-0.010	13.65
BaSO4	1.013e-08	1.013e-08	-7.994	-7.994	0.000	(0)
KSO4-	4.410e-09	4.305e-09	-8.356	-8.366	-0.010	34.09
MnSO4	1.160e-09	1.160e-09	-8.936	-8.936	0.000	22.54
CdSO4	6.925e-10	6.925e-10	-9.160	-9.160	0.000	78.05
PbSO4	1.324e-10	1.324e-10	-9.878	-9.878	0.000	(0)
HSO4-	1.117e-11	1.090e-11	-10.952	-10.962	-0.011	40.27
CuSO4	2.157e-12	2.158e-12	-11.666	-11.666	0.000	13.09
Cd(SO4)2-2	3.735e-13	3.390e-13	-12.428	-12.470	-0.042	-105.68
FeSO4	2.585e-13	2.585e-13	-12.588	-12.588	0.000	18.97
Pb(SO4)2-2	3.418e-14	3.103e-14	-13.466	-13.508	-0.042	(0)
CaHSO4+	1.196e-14	1.167e-14	-13.922	-13.933	-0.011	(0)
AlSO4+	7.410e-18	7.233e-18	-17.130	-17.141	-0.010	(0)
FeSO4+	1.559e-20	1.522e-20	-19.807	-19.818	-0.010	(0)
Al(SO4)2-	1.046e-20	1.021e-20	-19.980	-19.991	-0.010	(0)
FeHSO4+	4.373e-21	4.268e-21	-20.359	-20.370	-0.011	(0)
Fe(SO4)2-	1.523e-23	1.487e-23	-22.817	-22.828	-0.011	(0)
AlHSO4+2	1.775e-27	1.611e-27	-26.751	-26.793	-0.042	(0)
FeHSO4+2	1.128e-28	1.024e-28	-27.948	-27.990	-0.042	(0)
Si	4.644e-05					
H4SiO4	4.380e-05	4.381e-05	-4.359	-4.358	0.000	52.08
H3SiO4-	2.635e-06	2.571e-06	-5.579	-5.590	-0.011	27.96
H2SiO4-2	7.665e-11	6.964e-11	-10.115	-10.157	-0.042	(0)

-------------------------------Saturation indices--------------------------------

Phase	SI**	log IAP	log K(298 K, 1 atm)	
Al(OH)3(a)	-1.29	9.51	10.80	Al(OH)3
Albite	-3.94	-21.94	-18.00	NaAlSi3O8
Alunite	-9.43	-10.83	-1.40	KAl3(SO4)2(OH)6
Anglesite	-4.84	-12.63	-7.79	PbSO4

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  Anhydrite          -4.12     -8.40   -4.28  CaSO4
  Anorthite          -2.16    -21.88  -19.71  CaAl2Si2O8
  Aragonite          -1.54     -9.87   -8.34  CaCO3
  Barite             -0.72    -10.69   -9.97  BaSO4
  Ca-Montmorillonite  0.55    -44.48  -45.03  Ca0.165Al2.33Si3.67O10(OH)2
  Calcite            -1.39     -9.87   -8.48  CaCO3
  Cd(OH)2            -3.72      9.93   13.65  Cd(OH)2
  CdSiO3             -3.49      5.57    9.06  CdSiO3
  CdSO4             -11.52    -11.62   -0.10  CdSO4
  Cerrusite          -0.97    -14.10  -13.13  PbCO3
  Chalcedony         -0.81     -4.36   -3.55  SiO2
  Chlorite(14A)      -0.29     68.09   68.38  Mg5Al2Si3O10(OH)8
  Chrysotile         -3.63     28.57   32.20  Mg3Si2O5(OH)4
  CO2(g)             -4.88     -6.34   -1.46  CO2
  Dolomite           -3.38    -20.47  -17.09  CaMg(CO3)2
  Fe(OH)3(a)          1.40      6.29    4.89  Fe(OH)3
  Gibbsite            1.40      9.51    8.11  Al(OH)3
  Goethite            7.29      6.29   -1.00  FeOOH
  Gypsum             -3.82     -8.40   -4.58  CaSO4:2H2O
  H2(g)             -25.25    -28.35   -3.10  H2
  H2O(g)             -1.50     -0.00    1.50  H2O
  Halite            -10.25     -8.68    1.57  NaCl
  Hausmannite        -4.74     56.29   61.03  Mn3O4
  Hematite           16.59     12.59   -4.01  Fe2O3
  Illite              0.10    -40.16  -40.27  K0.6Mg0.25Al2.3Si3.5O10(OH)2
  Jarosite-K        -11.27    -20.48   -9.21  KFe3(SO4)2(OH)6
  K-feldspar         -1.92    -22.49  -20.57  KAlSi3O8
  K-mica              6.49     19.19   12.70  KAl3Si3O10(OH)2
  Kaolinite           2.87     10.30    7.43  Al2Si2O5(OH)4
  Manganite          -2.38     22.96   25.34  MnOOH
  Melanterite       -12.63    -14.84   -2.21  FeSO4:7H2O
  O2(g)              -0.91     -3.81   -2.89  O2
  Otavite            -0.99    -13.09  -12.10  CdCO3
  Pb(OH)2             0.77      8.92    8.15  Pb(OH)2
  Pyrochroite        -4.84     10.36   15.20  Mn(OH)2
  Pyrolusite         -5.82     35.56   41.38  MnO2:H2O
  Quartz             -0.38     -4.36   -3.98  SiO2
  Rhodochrosite      -1.53    -12.66  -11.13  MnCO3
  Sepiolite          -3.98     11.78   15.76  Mg2Si3O7.5OH:3H2O
  Sepiolite(d)       -6.88     11.78   18.66  Mg2Si3O7.5OH:3H2O
  Siderite           -5.42    -16.31  -10.89  FeCO3
  SiO2(a)            -1.65     -4.36   -2.71  SiO2
  Sylvite           -10.13     -9.23    0.90  KCl
  Talc               -1.54     19.86   21.40  Mg3Si4O10(OH)2
  Witherite          -3.60    -12.17   -8.56  BaCO3

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
  For ideal gases, phi = 1.

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End of simulation.
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Reading input data for simulation 3.
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      TITLE Aqua Mix part III: mix 75% soln 1, 25% soln 2.
      MIX 1
              1      0.75
              2      0.25
      SAVE solution   3
      END
-----
TITLE
-----

 Aqua Mix part III: mix 75% soln 1, 25% soln 2.
```

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----------------------------------------
Beginning of batch-reaction calculations.
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Reaction step 1.

Using mix 1.

Mixture 1.

        7.500e-01 Solution 1  MW-4
        2.500e-01 Solution 2  DI Extraction

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

      Elements           Molality       Moles

      Al                8.525e-06   8.525e-06
      Ba                5.098e-07   5.098e-07
      C                 1.685e-03   1.685e-03
      Ca                7.671e-04   7.671e-04
      Cd                1.557e-08   1.557e-08
      Cl                3.157e-04   3.157e-04
      Cu                5.509e-07   5.509e-07
      Fe                1.880e-07   1.880e-07
      K                 7.585e-05   7.585e-05
      Mg                1.297e-04   1.297e-04
      Mn                4.551e-08   4.551e-08
      Na                9.393e-04   9.393e-04
      Pb                1.424e-07   1.424e-07
      S                 2.686e-04   2.686e-04
      Si                1.641e-04   1.641e-04

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

                                     pH  =   7.873      Charge balance
                                     pe  =  13.436      Adjusted to redox equilibrium
       Specific Conductance (µS/cm, 16°C)  = 220
                            Density (g/cm³)  =   0.99900
                                 Volume (L)  =   1.00122
                          Activity of water  =   1.000
                             Ionic strength  =   3.705e-03
                         Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   1.680e-03
                        Total CO2 (mol/kg)  =   1.685e-03
                          Temperature (°C)  =  16.68
                   Electrical balance (eq)  =   3.038e-04
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   5.86
                                Iterations  =  16
                                   Total H  = 1.110147e+02
                                   Total O  = 5.551340e+01

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

                                                 Log       Log       Log    mole V
   Species          Molality    Activity  Molality  Activity     Gamma   cm³/mol

   OH-             4.156e-07   3.891e-07    -6.381    -6.410    -0.029     -4.49
   H+              1.424e-08   1.341e-08    -7.847    -7.873    -0.026      0.00
   H2O             5.551e+01   9.999e-01     1.744    -0.000     0.000     18.04
Al            8.525e-06
   Al(OH)4-        8.452e-06   7.922e-06    -5.073    -5.101    -0.028       (0)
   Al(OH)3         6.181e-08   6.187e-08    -7.209    -7.209     0.000       (0)
   Al(OH)2+        1.148e-08   1.077e-08    -7.940    -7.968    -0.028       (0)
   AlOH+2          5.105e-11   3.958e-11   -10.292   -10.403    -0.111    -27.37
   Al+3            1.588e-13   9.275e-14   -12.799   -13.033    -0.234    -41.53
   AlSO4+          5.330e-14   4.996e-14   -13.273   -13.301    -0.028       (0)
```

Al(SO4)2-	3.084e-16	2.890e-16	-15.511	-15.539	-0.028	(0)
AlHSO4+2	7.232e-23	5.572e-23	-22.141	-22.254	-0.113	(0)
Ba	5.098e-07					
Ba+2	4.702e-07	3.626e-07	-6.328	-6.441	-0.113	-13.18
BaSO4	3.456e-08	3.459e-08	-7.461	-7.461	0.000	(0)
BaHCO3+	4.315e-09	4.043e-09	-8.365	-8.393	-0.028	(0)
BaCO3	6.943e-10	6.949e-10	-9.158	-9.158	0.000	-10.79
BaOH+	9.767e-13	9.160e-13	-12.010	-12.038	-0.028	(0)
C(-4)	0.000e+00					
CH4	0.000e+00	0.000e+00	-149.213	-149.212	0.000	32.22
C(4)	1.685e-03					
HCO3-	1.611e-03	1.512e-03	-2.793	-2.821	-0.028	23.99
CO2	5.155e-05	5.159e-05	-4.288	-4.287	0.000	31.34
CaHCO3+	1.005e-05	9.439e-06	-4.998	-5.025	-0.027	9.33
CO3-2	5.656e-06	4.385e-06	-5.247	-5.358	-0.111	-6.06
CaCO3	3.645e-06	3.648e-06	-5.438	-5.438	0.000	-14.63
MgHCO3+	1.767e-06	1.656e-06	-5.753	-5.781	-0.028	5.23
NaHCO3	7.836e-07	7.843e-07	-6.106	-6.106	0.000	1.80
MgCO3	3.547e-07	3.550e-07	-6.450	-6.450	0.000	-17.08
PbCO3	1.330e-07	1.331e-07	-6.876	-6.876	0.000	(0)
CuCO3	9.085e-08	9.093e-08	-7.042	-7.041	0.000	(0)
NaCO3-	4.973e-08	4.659e-08	-7.303	-7.332	-0.028	-1.92
MnCO3	8.753e-09	8.761e-09	-8.058	-8.057	0.000	(0)
BaHCO3+	4.315e-09	4.043e-09	-8.365	-8.393	-0.028	(0)
MnHCO3+	3.613e-09	3.389e-09	-8.442	-8.470	-0.028	(0)
CuHCO3+	3.123e-09	2.926e-09	-8.505	-8.534	-0.028	(0)
PbHCO3+	2.239e-09	2.098e-09	-8.650	-8.678	-0.028	(0)
Pb(CO3)2-2	1.903e-09	1.466e-09	-8.721	-8.834	-0.113	(0)
BaCO3	6.943e-10	6.949e-10	-9.158	-9.158	0.000	-10.79
Cu(CO3)2-2	6.514e-10	5.019e-10	-9.186	-9.299	-0.113	(0)
CdHCO3+	5.524e-10	5.175e-10	-9.258	-9.286	-0.028	(0)
CdCO3	3.767e-11	3.771e-11	-10.424	-10.424	0.000	(0)
Cd(CO3)2-2	6.785e-13	5.228e-13	-12.168	-12.282	-0.113	(0)
FeHCO3+	4.481e-19	4.199e-19	-18.349	-18.377	-0.028	(0)
FeCO3	2.919e-19	2.922e-19	-18.535	-18.534	0.000	(0)
Ca	7.671e-04					
Ca+2	7.353e-04	5.698e-04	-3.134	-3.244	-0.111	-18.18
CaSO4	1.807e-05	1.809e-05	-4.743	-4.743	0.000	7.15
CaHCO3+	1.005e-05	9.439e-06	-4.998	-5.025	-0.027	9.33
CaCO3	3.645e-06	3.648e-06	-5.438	-5.438	0.000	-14.63
CaOH+	7.525e-09	7.050e-09	-8.124	-8.152	-0.028	(0)
CaHSO4+	1.523e-12	1.427e-12	-11.817	-11.846	-0.028	(0)
Cd	1.557e-08					
Cd+2	1.405e-08	1.083e-08	-7.852	-7.966	-0.113	-19.13
CdSO4	5.636e-10	5.641e-10	-9.249	-9.249	0.000	82.70
CdHCO3+	5.524e-10	5.175e-10	-9.258	-9.286	-0.028	(0)
CdCl+	3.171e-10	2.971e-10	-9.499	-9.527	-0.028	3.44
CdOH+	3.797e-11	3.558e-11	-10.421	-10.449	-0.028	(0)
CdCO3	3.767e-11	3.771e-11	-10.424	-10.424	0.000	(0)
CdOHCl	7.615e-12	7.622e-12	-11.118	-11.118	0.000	(0)
Cd(SO4)2-2	1.610e-12	1.241e-12	-11.793	-11.906	-0.113	-111.84
Cd(CO3)2-2	6.785e-13	5.228e-13	-12.168	-12.282	-0.113	(0)
CdCl2	3.545e-13	3.548e-13	-12.450	-12.450	0.000	23.14
Cd(OH)2	2.686e-13	2.688e-13	-12.571	-12.571	0.000	(0)
CdCl3-	6.210e-17	5.818e-17	-16.207	-16.235	-0.028	76.08
Cd2OH+3	3.773e-18	2.099e-18	-17.423	-17.678	-0.255	(0)
Cd(OH)3-	2.400e-18	2.249e-18	-17.620	-17.648	-0.028	(0)
Cd(OH)4-2	1.939e-24	1.494e-24	-23.712	-23.826	-0.113	(0)
CdHS+	0.000e+00	0.000e+00	-144.909	-144.937	-0.028	(0)
Cd(HS)2	0.000e+00	0.000e+00	-285.720	-285.719	0.000	(0)
Cd(HS)3-	0.000e+00	0.000e+00	-430.653	-430.681	-0.028	(0)
Cd(HS)4-2	0.000e+00	0.000e+00	-575.520	-575.633	-0.113	(0)
Cl	3.157e-04					
Cl-	3.157e-04	2.957e-04	-3.501	-3.529	-0.028	17.79
CdCl+	3.171e-10	2.971e-10	-9.499	-9.527	-0.028	3.44
MnCl+	3.230e-11	3.030e-11	-10.491	-10.519	-0.028	-5.48
PbCl+	1.775e-11	1.663e-11	-10.751	-10.779	-0.028	7.62
CdOHCl	7.615e-12	7.622e-12	-11.118	-11.118	0.000	(0)

CuCl+	2.157e-12	2.020e-12	-11.666	-11.695	-0.028	3.10
CdCl2	3.545e-13	3.548e-13	-12.450	-12.450	0.000	23.14
PbCl2	9.137e-15	9.145e-15	-14.039	-14.039	0.000	34.21
MnCl2	3.907e-15	3.910e-15	-14.408	-14.408	0.000	97.45
CuCl2	2.922e-16	2.924e-16	-15.534	-15.534	0.000	20.09
CdCl3-	6.210e-17	5.818e-17	-16.207	-16.235	-0.028	76.08
PbCl3-	2.174e-18	2.037e-18	-17.663	-17.691	-0.028	64.82
MnCl3-	3.395e-19	3.184e-19	-18.469	-18.497	-0.028	43.68
FeCl+2	3.979e-20	3.079e-20	-19.400	-19.512	-0.111	(0)
CuCl2-	2.066e-21	1.936e-21	-20.685	-20.713	-0.028	(0)
FeCl+	1.210e-21	1.134e-21	-20.917	-20.946	-0.028	(0)
PbCl4-2	3.503e-22	2.699e-22	-21.456	-21.569	-0.113	99.90
CuCl3-	2.814e-22	2.636e-22	-21.551	-21.579	-0.028	(0)
FeCl2+	5.688e-23	5.335e-23	-22.245	-22.273	-0.028	(0)
CuCl3-2	1.134e-24	8.776e-25	-23.945	-24.057	-0.111	(0)
FeCl3	1.576e-27	1.577e-27	-26.802	-26.802	0.000	(0)
CuCl4-2	4.140e-28	3.203e-28	-27.383	-27.494	-0.111	(0)
Cu(1)	7.544e-20					
Cu+	7.337e-20	6.861e-20	-19.134	-19.164	-0.029	(0)
CuCl2-	2.066e-21	1.936e-21	-20.685	-20.713	-0.028	(0)
CuCl3-2	1.134e-24	8.776e-25	-23.945	-24.057	-0.111	(0)
Cu(2)	5.509e-07					
Cu(OH)2	4.481e-07	4.485e-07	-6.349	-6.348	0.000	(0)
CuCO3	9.085e-08	9.093e-08	-7.042	-7.041	0.000	(0)
Cu+2	4.968e-09	3.862e-09	-8.304	-8.413	-0.109	-26.47
CuHCO3+	3.123e-09	2.926e-09	-8.505	-8.534	-0.028	(0)
CuOH+	3.073e-09	2.879e-09	-8.512	-8.541	-0.028	(0)
Cu(CO3)2-2	6.514e-10	5.019e-10	-9.186	-9.299	-0.113	(0)
CuSO4	1.413e-10	1.415e-10	-9.850	-9.849	0.000	11.92
CuCl+	2.157e-12	2.020e-12	-11.666	-11.695	-0.028	3.10
Cu(OH)3-	2.150e-12	2.015e-12	-11.668	-11.696	-0.028	(0)
Cu2(OH)2+2	2.011e-12	1.550e-12	-11.697	-11.810	-0.113	(0)
CuCl2	2.922e-16	2.924e-16	-15.534	-15.534	0.000	20.09
Cu(OH)4-2	3.889e-17	2.997e-17	-16.410	-16.523	-0.113	(0)
CuCl3-	2.814e-22	2.636e-22	-21.551	-21.579	-0.028	(0)
CuCl4-2	4.140e-28	3.203e-28	-27.383	-27.494	-0.111	(0)
Cu(HS)3-	0.000e+00	0.000e+00	-423.911	-423.939	-0.028	(0)
Fe(2)	4.432e-18					
Fe+2	3.573e-18	2.778e-18	-17.447	-17.556	-0.109	-22.63
FeHCO3+	4.481e-19	4.199e-19	-18.349	-18.377	-0.028	(0)
FeCO3	2.919e-19	2.922e-19	-18.535	-18.534	0.000	(0)
FeSO4	8.033e-20	8.040e-20	-19.095	-19.095	0.000	28.85
FeOH+	3.682e-20	3.453e-20	-19.434	-19.462	-0.028	(0)
FeCl+	1.210e-21	1.134e-21	-20.917	-20.946	-0.028	(0)
Fe(OH)2	1.040e-23	1.040e-23	-22.983	-22.983	0.000	(0)
Fe(OH)3-	2.825e-26	2.649e-26	-25.549	-25.577	-0.028	(0)
FeHSO4+	7.425e-27	6.957e-27	-26.129	-26.158	-0.028	(0)
Fe(HS)2	0.000e+00	0.000e+00	-302.891	-302.890	0.000	(0)
Fe(HS)3-	0.000e+00	0.000e+00	-447.967	-447.995	-0.028	(0)
Fe(3)	1.880e-07					
Fe(OH)3	1.550e-07	1.552e-07	-6.810	-6.809	0.000	(0)
Fe(OH)2+	2.501e-08	2.347e-08	-7.602	-7.630	-0.028	(0)
Fe(OH)4-	7.970e-09	7.478e-09	-8.099	-8.126	-0.028	(0)
FeOH+2	1.700e-12	1.315e-12	-11.770	-11.881	-0.111	(0)
FeSO4+	8.330e-18	7.813e-18	-17.079	-17.107	-0.028	(0)
Fe+3	7.749e-18	4.524e-18	-17.111	-17.344	-0.234	(0)
FeCl+2	3.979e-20	3.079e-20	-19.400	-19.512	-0.111	(0)
Fe(SO4)2-	3.358e-20	3.147e-20	-19.474	-19.502	-0.028	(0)
Fe2(OH)2+4	1.882e-22	6.634e-23	-21.725	-22.178	-0.453	(0)
FeCl2+	5.688e-23	5.335e-23	-22.245	-22.273	-0.028	(0)
FeHSO4+2	3.694e-25	2.846e-25	-24.433	-24.546	-0.113	(0)
Fe3(OH)4+5	3.656e-27	7.169e-28	-26.437	-27.145	-0.708	(0)
FeCl3	1.576e-27	1.577e-27	-26.802	-26.802	0.000	(0)
H(0)	0.000e+00					
H2	0.000e+00	0.000e+00	-45.730	-45.729	0.000	28.62
K	7.585e-05					
K+	7.576e-05	7.094e-05	-4.121	-4.149	-0.029	8.73
KSO4-	8.708e-08	8.171e-08	-7.060	-7.088	-0.028	33.87

Mg	1.297e-04					
Mg+2	1.241e-04	9.643e-05	-3.906	-4.016	-0.110	-21.42
MgSO4	3.448e-06	3.451e-06	-5.462	-5.462	0.000	5.48
MgHCO3+	1.767e-06	1.656e-06	-5.753	-5.781	-0.028	5.23
MgCO3	3.547e-07	3.550e-07	-6.450	-6.450	0.000	-17.08
MgOH+	1.282e-08	1.205e-08	-7.892	-7.919	-0.027	(0)
Mn(2)	4.551e-08					
Mn+2	3.236e-08	2.515e-08	-7.490	-7.599	-0.109	-20.61
MnCO3	8.753e-09	8.761e-09	-8.058	-8.057	0.000	(0)
MnHCO3+	3.613e-09	3.389e-09	-8.442	-8.470	-0.028	(0)
MnSO4	7.225e-10	7.232e-10	-9.141	-9.141	0.000	26.71
MnCl+	3.230e-11	3.030e-11	-10.491	-10.519	-0.028	-5.48
MnOH+	2.557e-11	2.398e-11	-10.592	-10.620	-0.028	(0)
MnCl2	3.907e-15	3.910e-15	-14.408	-14.408	0.000	97.45
MnCl3-	3.395e-19	3.184e-19	-18.469	-18.497	-0.028	43.68
Mn(OH)3-	1.761e-19	1.652e-19	-18.754	-18.782	-0.028	(0)
Mn(3)	1.039e-20					
Mn+3	1.039e-20	6.068e-21	-19.983	-20.217	-0.234	(0)
Na	9.393e-04					
Na+	9.376e-04	8.790e-04	-3.028	-3.056	-0.028	-1.93
NaSO4-	8.465e-07	7.943e-07	-6.072	-6.100	-0.028	14.16
NaHCO3	7.836e-07	7.843e-07	-6.106	-6.106	0.000	1.80
NaCO3-	4.973e-08	4.659e-08	-7.303	-7.332	-0.028	-1.92
NaOH	3.417e-20	3.420e-20	-19.466	-19.466	0.000	(0)
O(0)	4.124e-04					
O2	2.062e-04	2.064e-04	-3.686	-3.685	0.000	29.67
Pb	1.424e-07					
PbCO3	1.330e-07	1.331e-07	-6.876	-6.876	0.000	(0)
PbOH+	2.711e-09	2.540e-09	-8.567	-8.595	-0.028	(0)
Pb+2	2.267e-09	1.747e-09	-8.644	-8.758	-0.113	-15.38
PbHCO3+	2.239e-09	2.098e-09	-8.650	-8.678	-0.028	(0)
Pb(CO3)2-2	1.903e-09	1.466e-09	-8.721	-8.834	-0.113	(0)
PbSO4	1.869e-10	1.870e-10	-9.728	-9.728	0.000	(0)
Pb(OH)2	7.360e-11	7.367e-11	-10.133	-10.133	0.000	(0)
PbCl+	1.775e-11	1.663e-11	-10.751	-10.779	-0.028	7.62
Pb(SO4)2-2	2.425e-13	1.868e-13	-12.615	-12.729	-0.113	(0)
Pb(OH)3-	6.730e-14	6.306e-14	-13.172	-13.200	-0.028	(0)
PbCl2	9.137e-15	9.145e-15	-14.039	-14.039	0.000	34.21
Pb2OH+3	1.786e-16	9.934e-17	-15.748	-16.003	-0.255	(0)
Pb(OH)4-2	1.398e-17	1.077e-17	-16.855	-16.968	-0.113	(0)
PbCl3-	2.174e-18	2.037e-18	-17.663	-17.691	-0.028	64.82
Pb3(OH)4+2	7.801e-20	6.011e-20	-19.108	-19.221	-0.113	(0)
PbCl4-2	3.503e-22	2.699e-22	-21.456	-21.569	-0.113	99.90
Pb(HS)2	0.000e+00	0.000e+00	-287.772	-287.772	0.000	(0)
Pb(HS)3-	0.000e+00	0.000e+00	-433.585	-433.614	-0.028	(0)
S(-2)	0.000e+00					
CdHS+	0.000e+00	0.000e+00	-144.909	-144.937	-0.028	(0)
HS-	0.000e+00	0.000e+00	-147.113	-147.142	-0.029	20.17
H2S	0.000e+00	0.000e+00	-147.956	-147.956	0.000	37.13
S-2	0.000e+00	0.000e+00	-152.331	-152.442	-0.111	(0)
Cd(HS)2	0.000e+00	0.000e+00	-285.720	-285.719	0.000	(0)
Pb(HS)2	0.000e+00	0.000e+00	-287.772	-287.772	0.000	(0)
Fe(HS)2	0.000e+00	0.000e+00	-302.891	-302.890	0.000	(0)
Cu(HS)3-	0.000e+00	0.000e+00	-423.911	-423.939	-0.028	(0)
Cd(HS)3-	0.000e+00	0.000e+00	-430.653	-430.681	-0.028	(0)
Pb(HS)3-	0.000e+00	0.000e+00	-433.585	-433.614	-0.028	(0)
Fe(HS)3-	0.000e+00	0.000e+00	-447.967	-447.995	-0.028	(0)
Cd(HS)4-2	0.000e+00	0.000e+00	-575.520	-575.633	-0.113	(0)
S(6)	2.686e-04					
SO4-2	2.461e-04	1.904e-04	-3.609	-3.720	-0.112	13.32
CaSO4	1.807e-05	1.809e-05	-4.743	-4.743	0.000	7.15
MgSO4	3.448e-06	3.451e-06	-5.462	-5.462	0.000	5.48
NaSO4-	8.465e-07	7.943e-07	-6.072	-6.100	-0.028	14.16
KSO4-	8.708e-08	8.171e-08	-7.060	-7.088	-0.028	33.87
BaSO4	3.456e-08	3.459e-08	-7.461	-7.461	0.000	(0)
MnSO4	7.225e-10	7.232e-10	-9.141	-9.141	0.000	26.71
CdSO4	5.636e-10	5.641e-10	-9.249	-9.249	0.000	82.70
HSO4-	2.223e-10	2.083e-10	-9.653	-9.681	-0.028	39.64

PbSO4	1.869e-10	1.870e-10	-9.728	-9.728	0.000	(0)
CuSO4	1.413e-10	1.415e-10	-9.850	-9.849	0.000	11.92
Cd(SO4)2-2	1.610e-12	1.241e-12	-11.793	-11.906	-0.113	-111.84
CaHSO4+	1.523e-12	1.427e-12	-11.817	-11.846	-0.028	(0)
Pb(SO4)2-2	2.425e-13	1.868e-13	-12.615	-12.729	-0.113	(0)
AlSO4+	5.330e-14	4.996e-14	-13.273	-13.301	-0.028	(0)
Al(SO4)2-	3.084e-16	2.890e-16	-15.511	-15.539	-0.028	(0)
FeSO4+	8.330e-18	7.813e-18	-17.079	-17.107	-0.028	(0)
FeSO4	8.033e-20	8.040e-20	-19.095	-19.095	0.000	28.85
Fe(SO4)2-	3.358e-20	3.147e-20	-19.474	-19.502	-0.028	(0)
AlHSO4+2	7.232e-23	5.572e-23	-22.141	-22.254	-0.113	(0)
FeHSO4+2	3.694e-25	2.846e-25	-24.433	-24.546	-0.113	(0)
FeHSO4+	7.425e-27	6.957e-27	-26.129	-26.158	-0.028	(0)
Si	1.641e-04					
H4SiO4	1.627e-04	1.628e-04	-3.789	-3.788	0.000	52.87
H3SiO4-	1.407e-06	1.318e-06	-5.852	-5.880	-0.028	27.74
H2SiO4-2	4.878e-12	3.782e-12	-11.312	-11.422	-0.111	(0)

----------Saturation indices----------

Phase	SI**	log IAP	log K(289 K, 1 atm)	
Al(OH)3(a)	-0.77	10.58	11.36	Al(OH)3
Albite	-0.97	-19.52	-18.55	NaAlSi3O8
Alunite	-3.11	-3.45	-0.34	KAl3(SO4)2(OH)6
Anglesite	-4.64	-12.48	-7.84	PbSO4
Anhydrite	-2.78	-6.96	-4.19	CaSO4
Anorthite	-1.07	-21.02	-19.96	CaAl2Si2O8
Aragonite	-0.31	-8.60	-8.29	CaCO3
Barite	-0.05	-10.16	-10.11	BaSO4
Ca-Montmorillonite	4.19	-42.07	-46.26	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	-0.16	-8.60	-8.44	CaCO3
Cd(OH)2	-5.87	7.78	13.65	Cd(OH)2
CdSiO3	-5.42	3.99	9.41	CdSiO3
CdSO4	-11.90	-11.69	0.21	CdSO4
Cerrusite	-0.88	-14.12	-13.23	PbCO3
CH4(g)	-146.44	-149.21	-2.77	CH4
Chalcedony	-0.14	-3.79	-3.65	SiO2
Chlorite(14A)	-3.12	68.45	71.57	Mg5Al2Si3O10(OH)8
Chrysotile	-5.65	27.61	33.26	Mg3Si2O5(OH)4
CO2(g)	-2.93	-4.29	-1.36	CO2
Dolomite	-1.08	-17.98	-16.89	CaMg(CO3)2
Fe(OH)3(a)	1.38	6.27	4.89	Fe(OH)3
FeS(ppt)	-152.91	-156.83	-3.92	FeS
Gibbsite	1.99	10.58	8.59	Al(OH)3
Goethite	6.97	6.27	-0.70	FeOOH
Gypsum	-2.38	-6.96	-4.58	CaSO4:2H2O
H2(g)	-42.65	-45.73	-3.08	H2
H2O(g)	-1.72	-0.00	1.72	H2O
H2S(g)	-147.00	-155.01	-8.01	H2S
Halite	-8.15	-6.59	1.56	NaCl
Hausmannite	3.90	67.05	63.15	Mn3O4
Hematite	15.90	12.55	-3.36	Fe2O3
Illite	3.49	-37.93	-41.42	K0.6Mg0.25Al2.3Si3.5O10(OH)2
Jarosite-K	-7.84	-16.39	-8.55	KFe3(SO4)2(OH)6
K-feldspar	0.61	-20.62	-21.22	KAlSi3O8
K-mica	10.16	24.11	13.95	KAl3Si3O10(OH)2
Kaolinite	5.41	13.59	8.18	Al2Si2O5(OH)4
Mackinawite	-152.18	-156.83	-4.65	FeS
Manganite	4.11	29.45	25.34	MnOOH
Melanterite	-18.96	-21.28	-2.32	FeSO4:7H2O
O2(g)	-0.86	-3.69	-2.83	O2
Otavite	-1.22	-13.32	-12.10	CdCO3
Pb(OH)2	-1.46	6.99	8.44	Pb(OH)2
Pyrite	-250.51	-269.22	-18.72	FeS2
Pyrochroite	-7.05	8.15	15.20	Mn(OH)2
Pyrolusite	8.01	50.76	42.75	MnO2:H2O
Quartz	0.32	-3.79	-4.11	SiO2

Rhodochrosite	-1.86	-12.96	-11.10	MnCO3
Sepiolite	-3.89	12.09	15.99	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-6.57	12.09	18.66	Mg2Si3O7.5OH:3H2O
Siderite	-12.08	-22.91	-10.84	FeCO3
SiO2(a)	-1.01	-3.79	-2.78	SiO2
Sulfur	-110.42	-105.34	5.08	S
Sylvite	-8.54	-7.68	0.86	KCl
Talc	-2.34	20.03	22.37	Mg3Si4O10(OH)2
Witherite	-3.21	-11.80	-8.59	BaCO3

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 4.

End of Run after 0.24 Seconds.

```
   Input file: E:\Project Stuff\Models\Mixing 50_50.pqi
  Output file: E:\Project Stuff\Models\Mixing 50_50.pqo
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.2.2-10160\database
\phreeqc.dat

------------------
Reading data base.
------------------

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

      DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 3.2.2-10160\database
\phreeqc.dat
      TITLE Water Mixing Scenario Part I
      SOLUTION 1  MW-4
            units   ppm
            temp    13.9
            pH    7.87
            O(0)            7.13
            Ca              39.66
            Mg              4.05
            Na              28.4
            K               3.77
            Ba              0.07
            Be              0
            Cd              0
            Cu              0.03
            Pb              0.026
            Mn              0
            Se              0
            Ni              0.011
            Fe              0
            Al              0.05
            As              0
            Cl              14.4
            Alkalinity      132.4 as HCO3
            S(6)        32.79
            Si    12.21
      SAVE solution 1
      END
-----
TITLE
-----

 Water Mixing Scenario Part I

WARNING: Could not find element in database, As.
      Concentration is set to zero.
WARNING: Could not find element in database, Be.
      Concentration is set to zero.
WARNING: Could not find element in database, Ni.
      Concentration is set to zero.
WARNING: Could not find element in database, Se.
      Concentration is set to zero.
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------
```

Initial solution 1. MW-4

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

Elements	Molality	Moles
Al	1.854e-06	1.854e-06
Alkalinity	2.170e-03	2.170e-03
Ba	5.098e-07	5.098e-07
Ca	9.898e-04	9.898e-04
Cl	4.063e-04	4.063e-04
Cu	4.722e-07	4.722e-07
K	9.644e-05	9.644e-05
Mg	1.666e-04	1.666e-04
Na	1.236e-03	1.236e-03
O(0)	4.457e-04	4.457e-04
Pb	1.255e-07	1.255e-07
S(6)	3.414e-04	3.414e-04
Si	2.033e-04	2.033e-04

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

pH	= 7.870
pe	= 4.000
Specific Conductance (µS/cm, 13°C)	= 262
Density (g/cm³)	= 0.99948
Volume (L)	= 1.00080
Activity of water	= 1.000
Ionic strength	= 4.770e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 2.218e-03
Total CO2 (mol/kg)	= 2.218e-03
Temperature (°C)	= 13.90
Electrical balance (eq)	= 3.932e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 5.86
Iterations	= 9
Total H	= 1.110154e+02
Total O	= 5.551543e+01

----------Redox couples----------

Redox couple	pe	Eh (volts)
O(-2)/O(0)	13.6923	0.7798

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	3.297e-07	3.063e-07	-6.482	-6.514	-0.032	-4.67
H+	1.441e-08	1.349e-08	-7.841	-7.870	-0.029	0.00
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.03
Al	1.854e-06					
Al(OH)4-	1.837e-06	1.709e-06	-5.736	-5.767	-0.031	(0)
Al(OH)3	1.370e-08	1.371e-08	-7.863	-7.863	0.000	(0)
Al(OH)2+	3.254e-09	3.031e-09	-8.488	-8.518	-0.031	(0)
AlOH+2	1.953e-11	1.470e-11	-10.709	-10.833	-0.123	-27.24
Al+3	7.592e-14	4.184e-14	-13.120	-13.378	-0.259	-41.29
AlSO4+	2.836e-14	2.638e-14	-13.547	-13.579	-0.031	(0)
Al(SO4)2-	1.968e-16	1.830e-16	-15.706	-15.737	-0.031	(0)
AlHSO4+2	3.893e-23	2.909e-23	-22.410	-22.536	-0.127	(0)
Ba	5.098e-07					
Ba+2	4.639e-07	3.469e-07	-6.334	-6.460	-0.126	-13.38
BaSO4	4.021e-08	4.025e-08	-7.396	-7.395	0.000	(0)
BaHCO3+	4.968e-09	4.618e-09	-8.304	-8.336	-0.032	(0)
BaCO3	7.578e-10	7.587e-10	-9.120	-9.120	0.000	-10.82

BaOH+	9.360e-13	8.714e-13	-12.029	-12.060	-0.031	(0)
C(4)	2.218e-03					
HCO3-	2.115e-03	1.970e-03	-2.675	-2.706	-0.031	23.69
CO2	7.110e-05	7.118e-05	-4.148	-4.148	0.000	32.23
CaHCO3+	1.541e-05	1.436e-05	-4.812	-4.843	-0.030	9.19
CO3-2	7.027e-06	5.290e-06	-5.153	-5.277	-0.123	-6.47
CaCO3	5.292e-06	5.298e-06	-5.276	-5.276	0.000	-14.64
MgHCO3+	2.860e-06	2.659e-06	-5.544	-5.575	-0.032	5.12
NaHCO3	1.355e-06	1.356e-06	-5.868	-5.868	0.000	1.80
MgCO3	5.085e-07	5.091e-07	-6.294	-6.293	0.000	-17.08
PbCO3	1.174e-07	1.175e-07	-6.931	-6.930	0.000	(0)
CuCO3	9.142e-08	9.152e-08	-7.039	-7.038	0.000	(0)
NaCO3-	6.795e-08	6.318e-08	-7.168	-7.199	-0.032	-2.32
BaHCO3+	4.968e-09	4.618e-09	-8.304	-8.336	-0.032	(0)
CuHCO3+	3.421e-09	3.180e-09	-8.466	-8.498	-0.032	(0)
PbHCO3+	2.150e-09	1.999e-09	-8.667	-8.699	-0.032	(0)
Pb(CO3)2-2	2.089e-09	1.561e-09	-8.680	-8.807	-0.127	(0)
Cu(CO3)2-2	8.157e-10	6.095e-10	-9.088	-9.215	-0.127	(0)
BaCO3	7.578e-10	7.587e-10	-9.120	-9.120	0.000	-10.82
Ca	9.898e-04					
Ca+2	9.423e-04	7.090e-04	-3.026	-3.149	-0.124	-18.22
CaSO4	2.674e-05	2.677e-05	-4.573	-4.572	0.000	7.01
CaHCO3+	1.541e-05	1.436e-05	-4.812	-4.843	-0.030	9.19
CaCO3	5.292e-06	5.298e-06	-5.276	-5.276	0.000	-14.64
CaOH+	9.381e-09	8.722e-09	-8.028	-8.059	-0.032	(0)
CaHSO4+	2.210e-12	2.055e-12	-11.656	-11.687	-0.032	(0)
Cl	4.063e-04					
Cl-	4.063e-04	3.775e-04	-3.391	-3.423	-0.032	17.65
PbCl+	1.552e-11	1.443e-11	-10.809	-10.841	-0.032	7.49
CuCl2-	7.565e-12	7.032e-12	-11.121	-11.153	-0.032	(0)
CuCl+	2.002e-12	1.861e-12	-11.698	-11.730	-0.032	4.07
PbCl2	1.070e-14	1.071e-14	-13.971	-13.970	0.000	33.91
CuCl3-2	5.359e-15	4.025e-15	-14.271	-14.395	-0.124	(0)
CuCl2	3.328e-16	3.332e-16	-15.478	-15.477	0.000	15.77
PbCl3-	3.217e-18	2.991e-18	-17.493	-17.524	-0.032	64.36
PbCl4-2	6.619e-22	4.946e-22	-21.179	-21.306	-0.127	99.29
CuCl3-	3.914e-22	3.638e-22	-21.407	-21.439	-0.032	(0)
CuCl4-2	7.018e-28	5.271e-28	-27.154	-27.278	-0.124	(0)
Cu(1)	1.713e-10					
Cu+	1.637e-10	1.518e-10	-9.786	-9.819	-0.033	(0)
CuCl2-	7.565e-12	7.032e-12	-11.121	-11.153	-0.032	(0)
CuCl3-2	5.359e-15	4.025e-15	-14.271	-14.395	-0.124	(0)
Cu(2)	4.721e-07					
Cu(OH)2	3.694e-07	3.698e-07	-6.432	-6.432	0.000	(0)
CuCO3	9.142e-08	9.152e-08	-7.039	-7.038	0.000	(0)
Cu+2	4.265e-09	3.222e-09	-8.370	-8.492	-0.122	-26.44
CuHCO3+	3.421e-09	3.180e-09	-8.466	-8.498	-0.032	(0)
CuOH+	2.569e-09	2.388e-09	-8.590	-8.622	-0.032	(0)
Cu(CO3)2-2	8.157e-10	6.095e-10	-9.088	-9.215	-0.127	(0)
CuSO4	1.405e-10	1.406e-10	-9.852	-9.852	0.000	11.45
CuCl+	2.002e-12	1.861e-12	-11.698	-11.730	-0.032	4.07
Cu(OH)3-	1.777e-12	1.652e-12	-11.750	-11.782	-0.032	(0)
Cu2(OH)2+2	1.063e-12	7.943e-13	-11.973	-12.100	-0.127	(0)
CuCl2	3.328e-16	3.332e-16	-15.478	-15.477	0.000	15.77
Cu(OH)4-2	3.269e-17	2.443e-17	-16.486	-16.612	-0.127	(0)
CuCl3-	3.914e-22	3.638e-22	-21.407	-21.439	-0.032	(0)
CuCl4-2	7.018e-28	5.271e-28	-27.154	-27.278	-0.124	(0)
H(0)	2.887e-27					
H2	1.443e-27	1.445e-27	-26.841	-26.840	0.000	28.62
K	9.644e-05					
K+	9.631e-05	8.947e-05	-4.016	-4.048	-0.032	8.61
KSO4-	1.278e-07	1.190e-07	-6.894	-6.924	-0.031	33.76
Mg	1.666e-04					
Mg+2	1.584e-04	1.196e-04	-3.800	-3.922	-0.122	-21.29
MgSO4	4.817e-06	4.823e-06	-5.317	-5.317	0.000	5.34
MgHCO3+	2.860e-06	2.659e-06	-5.544	-5.575	-0.032	5.12
MgCO3	5.085e-07	5.091e-07	-6.294	-6.293	0.000	-17.08
MgOH+	1.218e-08	1.136e-08	-7.914	-7.944	-0.030	(0)

Na	1.236e-03					
Na+	1.233e-03	1.147e-03	-2.909	-2.940	-0.031	-2.12
NaHCO3	1.355e-06	1.356e-06	-5.868	-5.868	0.000	1.80
NaSO4-	1.328e-06	1.237e-06	-5.877	-5.908	-0.031	14.25
NaCO3-	6.795e-08	6.318e-08	-7.168	-7.199	-0.032	-2.32
NaOH	3.510e-20	3.514e-20	-19.455	-19.454	0.000	(0)
O(0)	4.457e-04					
O2	2.229e-04	2.231e-04	-3.652	-3.651	0.000	29.39
Pb	1.255e-07					
PbCO3	1.174e-07	1.175e-07	-6.931	-6.930	0.000	(0)
PbHCO3+	2.150e-09	1.999e-09	-8.667	-8.699	-0.032	(0)
Pb(CO3)2-2	2.089e-09	1.561e-09	-8.680	-8.807	-0.127	(0)
PbOH+	1.987e-09	1.847e-09	-8.702	-8.734	-0.032	(0)
Pb+2	1.710e-09	1.278e-09	-8.767	-8.893	-0.127	-15.34
PbSO4	1.662e-10	1.664e-10	-9.779	-9.779	0.000	(0)
Pb(OH)2	5.320e-11	5.326e-11	-10.274	-10.274	0.000	(0)
PbCl+	1.552e-11	1.443e-11	-10.809	-10.841	-0.032	7.49
Pb(SO4)2-2	2.705e-13	2.021e-13	-12.568	-12.694	-0.127	(0)
Pb(OH)3-	4.876e-14	4.533e-14	-13.312	-13.344	-0.032	(0)
PbCl2	1.070e-14	1.071e-14	-13.971	-13.970	0.000	33.91
Pb2OH+3	1.018e-16	5.284e-17	-15.992	-16.277	-0.285	(0)
Pb(OH)4-2	1.030e-17	7.697e-18	-16.987	-17.114	-0.127	(0)
PbCl3-	3.217e-18	2.991e-18	-17.493	-17.524	-0.032	64.36
Pb3(OH)4+2	1.972e-20	1.473e-20	-19.705	-19.832	-0.127	(0)
PbCl4-2	6.619e-22	4.946e-22	-21.179	-21.306	-0.127	99.29
S(6)	3.414e-04					
SO4-2	3.084e-04	2.315e-04	-3.511	-3.635	-0.125	12.78
CaSO4	2.674e-05	2.677e-05	-4.573	-4.572	0.000	7.01
MgSO4	4.817e-06	4.823e-06	-5.317	-5.317	0.000	5.34
NaSO4-	1.328e-06	1.237e-06	-5.877	-5.908	-0.031	14.25
KSO4-	1.278e-07	1.190e-07	-6.894	-6.924	-0.031	33.76
BaSO4	4.021e-08	4.025e-08	-7.396	-7.395	0.000	(0)
HSO4-	2.593e-10	2.411e-10	-9.586	-9.618	-0.032	39.37
PbSO4	1.662e-10	1.664e-10	-9.779	-9.779	0.000	(0)
CuSO4	1.405e-10	1.406e-10	-9.852	-9.852	0.000	11.45
CaHSO4+	2.210e-12	2.055e-12	-11.656	-11.687	-0.032	(0)
Pb(SO4)2-2	2.705e-13	2.021e-13	-12.568	-12.694	-0.127	(0)
AlSO4+	2.836e-14	2.638e-14	-13.547	-13.579	-0.031	(0)
Al(SO4)2-	1.968e-16	1.830e-16	-15.706	-15.737	-0.031	(0)
AlHSO4+2	3.893e-23	2.909e-23	-22.410	-22.536	-0.127	(0)
Si	2.033e-04					
H4SiO4	2.017e-04	2.019e-04	-3.695	-3.695	0.000	53.18
H3SiO4-	1.567e-06	1.457e-06	-5.805	-5.837	-0.032	27.62
H2SiO4-2	4.507e-12	3.393e-12	-11.346	-11.469	-0.123	(0)

----------Saturation indices----------

Phase	SI**	log IAP	log K(287 K, 1 atm)	
Al(OH)3(a)	-1.32	10.23	11.55	Al(OH)3
Albite	-1.06	-19.79	-18.74	NaAlSi3O8
Alunite	-4.26	-4.23	0.02	KAl3(SO4)2(OH)6
Anglesite	-4.68	-12.53	-7.85	PbSO4
Anhydrite	-2.62	-6.78	-4.16	CaSO4
Anorthite	-2.03	-22.07	-20.04	CaAl2Si2O8
Aragonite	-0.15	-8.43	-8.27	CaCO3
Barite	0.07	-10.10	-10.17	BaSO4
Ca-Montmorillonite	3.42	-43.26	-46.68	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	-0.00	-8.43	-8.43	CaCO3
Cerrusite	-0.90	-14.17	-13.27	PbCO3
Chalcedony	-0.01	-3.69	-3.69	SiO2
Chlorite(14A)	-4.21	68.47	72.67	Mg5Al2Si3O10(OH)8
Chrysotile	-5.56	28.06	33.63	Mg3Si2O5(OH)4
CO2(g)	-2.83	-4.15	-1.32	CO2
Dolomite	-0.80	-17.62	-16.82	CaMg(CO3)2
Gibbsite	1.48	10.23	8.76	Al(OH)3
Gypsum	-2.20	-6.78	-4.59	CaSO4:2H2O
H2(g)	-23.77	-26.84	-3.07	H2

```
  H2O(g)           -1.80     -0.00    1.80  H2O
  Halite           -7.92     -6.36    1.56  NaCl
  Illite            2.77    -39.05  -41.82  K0.6Mg0.25Al2.3Si3.5O10(OH)2
  K-feldspar        0.55    -20.90  -21.45  KAlSi3O8
  K-mica            9.05     23.43   14.39  KAl3Si3O10(OH)2
  Kaolinite         4.64     13.07    8.44  Al2Si2O5(OH)4
  O2(g)            -0.85     -3.65   -2.80  O2
  Pb(OH)2          -1.70      6.85    8.55  Pb(OH)2
  Quartz            0.46     -3.69   -4.15  SiO2
  Sepiolite        -3.51     12.55   16.06  Mg2Si3O7.5OH:3H2O
  Sepiolite(d)     -6.11     12.55   18.66  Mg2Si3O7.5OH:3H2O
  SiO2(a)          -0.89     -3.69   -2.81  SiO2
  Sylvite          -8.31     -7.47    0.84  KCl
  Talc             -2.04     20.67   22.71  Mg3Si4O10(OH)2
  Witherite        -3.13    -11.74   -8.60  BaCO3

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
  For ideal gases, phi = 1.

------------------
End of simulation.
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Reading input data for simulation 2.
-----------------------------------

      TITLE Mixing Scenario Part II
      SOLUTION 2  DI Extraction
            units   ppm
            temp    25.0
            pH    8.6
            O(0)            5.0
            Ca              3.97
            Mg              0.46
            Na              1.15
            K               0.55
            Ba              0.07
            Be              0.08
            Cd              0.007
            Cu              0.05
            Pb              0.04
            Mn              0.01
            Se              0.02
            Ni              0.01
            Fe              0.042
            Al              0.77
            As              0.04
            Cl              1.56
            Alkalinity      12.83 as HCO3
            S(6)        4.81
            Si    2.79
      END
-----
TITLE
-----

 Mixing Scenario Part II

WARNING: Could not find element in database, As.
      Concentration is set to zero.
WARNING: Could not find element in database, Be.
      Concentration is set to zero.
WARNING: Could not find element in database, Ni.
      Concentration is set to zero.
WARNING: Could not find element in database, Se.
      Concentration is set to zero.
-----------------------------------------
```

Beginning of initial solution calculations.

Initial solution 2. DI Extraction

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

Elements	Molality	Moles
Al	2.854e-05	2.854e-05
Alkalinity	2.103e-04	2.103e-04
Ba	5.097e-07	5.097e-07
Ca	9.906e-05	9.906e-05
Cd	6.228e-08	6.228e-08
Cl	4.400e-05	4.400e-05
Cu	7.869e-07	7.869e-07
Fe	7.521e-07	7.521e-07
K	1.407e-05	1.407e-05
Mg	1.892e-05	1.892e-05
Mn	1.820e-07	1.820e-07
Na	5.002e-05	5.002e-05
O(0)	3.125e-04	3.125e-04
Pb	1.931e-07	1.931e-07
S(6)	5.007e-05	5.007e-05
Si	4.644e-05	4.644e-05

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

pH	= 8.600
pe	= 4.000
Specific Conductance (µS/cm, 25°C)	= 32
Density (g/cm³)	= 0.99706
Volume (L)	= 1.00297
Activity of water	= 1.000
Ionic strength	= 4.496e-04
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 8.518e-05
Total CO2 (mol/kg)	= 8.518e-05
Temperature (°C)	= 25.00
Electrical balance (eq)	= 3.546e-05
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 6.30
Iterations	= 9
Total H	= 1.110128e+02
Total O	= 5.550729e+01

-----Redox couples-----

Redox couple	pe	Eh (volts)
O(-2)/O(0)	11.9685	0.7080

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	4.129e-06	4.029e-06	-5.384	-5.395	-0.011	-4.12
H+	2.571e-09	2.512e-09	-8.590	-8.600	-0.010	0.00
H2O	5.551e+01	1.000e+00	1.744	-0.000	0.000	18.07
Al	2.854e-05					
Al(OH)4-	2.850e-05	2.782e-05	-4.545	-4.556	-0.010	(0)
Al(OH)3	3.708e-08	3.708e-08	-7.431	-7.431	0.000	(0)
Al(OH)2+	6.475e-10	6.321e-10	-9.189	-9.199	-0.010	(0)
AlOH+2	2.230e-13	2.026e-13	-12.652	-12.693	-0.042	-27.80
Al+3	6.326e-17	5.123e-17	-16.199	-16.290	-0.092	-42.36
AlSO4+	7.410e-18	7.233e-18	-17.130	-17.141	-0.010	(0)
Al(SO4)2-	1.046e-20	1.021e-20	-19.980	-19.991	-0.010	(0)
AlHSO4+2	1.775e-27	1.611e-27	-26.751	-26.793	-0.042	(0)

Ba	5.097e-07					
Ba+2	4.989e-07	4.528e-07	-6.302	-6.344	-0.042	-12.78
BaSO4	1.013e-08	1.013e-08	-7.994	-7.994	0.000	(0)
BaHCO3+	3.584e-10	3.498e-10	-9.446	-9.456	-0.011	(0)
BaCO3	3.520e-10	3.520e-10	-9.454	-9.453	0.000	-10.70
BaOH+	6.257e-12	6.109e-12	-11.204	-11.214	-0.010	(0)
C(4)	8.518e-05					
HCO3-	8.254e-05	8.059e-05	-4.083	-4.094	-0.010	24.67
CO3-2	1.656e-06	1.505e-06	-5.781	-5.823	-0.042	-5.31
CO2	4.551e-07	4.551e-07	-6.342	-6.342	0.000	29.09
CaCO3	2.250e-07	2.251e-07	-6.648	-6.648	0.000	-14.60
PbCO3	1.379e-07	1.379e-07	-6.860	-6.860	0.000	(0)
CaHCO3+	9.377e-08	9.155e-08	-7.028	-7.038	-0.010	9.66
MgCO3	2.437e-08	2.437e-08	-7.613	-7.613	0.000	-17.09
MnCO3	1.746e-08	1.746e-08	-7.758	-7.758	0.000	(0)
MgHCO3+	1.640e-08	1.600e-08	-7.785	-7.796	-0.011	5.47
NaHCO3	2.212e-09	2.212e-09	-8.655	-8.655	0.000	1.80
CuCO3	1.912e-09	1.912e-09	-8.718	-8.718	0.000	(0)
NaCO3-	1.401e-09	1.368e-09	-8.853	-8.864	-0.011	-1.04
MnHCO3+	1.075e-09	1.049e-09	-8.969	-8.979	-0.010	(0)
Pb(CO3)2-2	5.742e-10	5.212e-10	-9.241	-9.283	-0.042	(0)
BaHCO3+	3.584e-10	3.498e-10	-9.446	-9.456	-0.011	(0)
BaCO3	3.520e-10	3.520e-10	-9.454	-9.453	0.000	-10.70
PbHCO3+	3.459e-10	3.376e-10	-9.461	-9.472	-0.011	(0)
CdHCO3+	1.404e-10	1.371e-10	-9.853	-9.863	-0.011	(0)
CdCO3	6.427e-11	6.428e-11	-10.192	-10.192	0.000	(0)
CuHCO3+	9.794e-12	9.560e-12	-11.009	-11.020	-0.011	(0)
Cu(CO3)2-2	3.991e-12	3.623e-12	-11.399	-11.441	-0.042	(0)
FeCO3	1.175e-12	1.175e-12	-11.930	-11.930	0.000	(0)
Cd(CO3)2-2	3.369e-13	3.058e-13	-12.472	-12.515	-0.042	(0)
FeHCO3+	2.688e-13	2.624e-13	-12.571	-12.581	-0.011	(0)
Ca	9.906e-05					
Ca+2	9.802e-05	8.904e-05	-4.009	-4.050	-0.042	-18.18
CaSO4	7.069e-07	7.070e-07	-6.151	-6.151	0.000	7.50
CaCO3	2.250e-07	2.251e-07	-6.648	-6.648	0.000	-14.60
CaHCO3+	9.377e-08	9.155e-08	-7.028	-7.038	-0.010	9.66
CaOH+	6.027e-09	5.883e-09	-8.220	-8.230	-0.011	(0)
CaHSO4+	1.196e-14	1.167e-14	-13.922	-13.933	-0.011	(0)
Cd	6.228e-08					
Cd+2	5.926e-08	5.378e-08	-7.227	-7.269	-0.042	-18.79
CdOH+	1.825e-09	1.781e-09	-8.739	-8.749	-0.011	(0)
CdSO4	6.925e-10	6.925e-10	-9.160	-9.160	0.000	78.05
CdCl+	2.260e-10	2.206e-10	-9.646	-9.656	-0.011	5.82
CdHCO3+	1.404e-10	1.371e-10	-9.853	-9.863	-0.011	(0)
CdCO3	6.427e-11	6.428e-11	-10.192	-10.192	0.000	(0)
Cd(OH)2	3.807e-11	3.808e-11	-10.419	-10.419	0.000	(0)
CdOHCl	3.627e-11	3.627e-11	-10.440	-10.440	0.000	(0)
Cd(SO4)2-2	3.735e-13	3.390e-13	-12.428	-12.470	-0.042	-105.68
Cd(CO3)2-2	3.369e-13	3.058e-13	-12.472	-12.515	-0.042	(0)
CdCl2	3.949e-14	3.949e-14	-13.404	-13.403	0.000	23.14
Cd(OH)3-	1.742e-15	1.701e-15	-14.759	-14.769	-0.011	(0)
Cd2OH+3	5.834e-16	4.691e-16	-15.234	-15.329	-0.095	(0)
CdCl3-	1.096e-18	1.070e-18	-17.960	-17.971	-0.011	69.31
Cd(OH)4-2	6.648e-21	6.034e-21	-20.177	-20.219	-0.042	(0)
Cl	4.400e-05					
Cl-	4.400e-05	4.295e-05	-4.357	-4.367	-0.011	18.06
CdCl+	2.260e-10	2.206e-10	-9.646	-9.656	-0.011	5.82
CdOHCl	3.627e-11	3.627e-11	-10.440	-10.440	0.000	(0)
MnCl+	2.619e-11	2.556e-11	-10.582	-10.592	-0.010	-3.10
PbCl+	9.239e-12	9.017e-12	-11.034	-11.045	-0.011	7.94
CdCl2	3.949e-14	3.949e-14	-13.404	-13.403	0.000	23.14
CuCl+	2.803e-14	2.736e-14	-13.552	-13.563	-0.011	0.62
CuCl2-	7.423e-15	7.246e-15	-14.129	-14.140	-0.011	(0)
FeCl+	1.978e-15	1.930e-15	-14.704	-14.714	-0.011	(0)
PbCl2	6.137e-16	6.138e-16	-15.212	-15.212	0.000	34.97
MnCl2	4.792e-16	4.793e-16	-15.319	-15.319	0.000	85.89
CdCl3-	1.096e-18	1.070e-18	-17.960	-17.971	-0.011	69.31
CuCl2	6.310e-19	6.311e-19	-18.200	-18.200	0.000	31.02

CuCl3-2	5.430e-19	4.932e-19	-18.265	-18.307	-0.042	(0)
PbCl3-	2.145e-20	2.094e-20	-19.669	-19.679	-0.011	65.94
MnCl3-	5.807e-21	5.669e-21	-20.236	-20.246	-0.010	43.34
FeCl+2	4.441e-23	4.033e-23	-22.353	-22.394	-0.042	(0)
PbCl4-2	4.742e-25	4.304e-25	-24.324	-24.366	-0.042	101.31
CuCl3-	9.852e-26	9.616e-26	-25.006	-25.017	-0.011	(0)
FeCl2+	7.925e-27	7.737e-27	-26.101	-26.111	-0.010	(0)
FeCl3	3.323e-32	3.323e-32	-31.479	-31.478	0.000	(0)
CuCl4-2	2.279e-32	2.070e-32	-31.642	-31.684	-0.042	(0)
Cu(1)	1.274e-11					
Cu+	1.273e-11	1.242e-11	-10.895	-10.906	-0.011	(0)
CuCl2-	7.423e-15	7.246e-15	-14.129	-14.140	-0.011	(0)
CuCl3-2	5.430e-19	4.932e-19	-18.265	-18.307	-0.042	(0)
Cu(2)	7.868e-07					
Cu(OH)2	7.837e-07	7.838e-07	-6.106	-6.106	0.000	(0)
CuCO3	1.912e-09	1.912e-09	-8.718	-8.718	0.000	(0)
CuOH+	9.654e-10	9.423e-10	-9.015	-9.026	-0.011	(0)
Cu+2	2.604e-10	2.367e-10	-9.584	-9.626	-0.042	-26.64
Cu(OH)3-	1.926e-11	1.880e-11	-10.715	-10.726	-0.011	(0)
CuHCO3+	9.794e-12	9.560e-12	-11.009	-11.020	-0.011	(0)
Cu(CO3)2-2	3.991e-12	3.623e-12	-11.399	-11.441	-0.042	(0)
CuSO4	2.157e-12	2.158e-12	-11.666	-11.666	0.000	13.09
Cu2(OH)2+2	4.281e-13	3.885e-13	-12.368	-12.411	-0.042	(0)
CuCl+	2.803e-14	2.736e-14	-13.552	-13.563	-0.011	0.62
Cu(OH)4-2	1.645e-15	1.493e-15	-14.784	-14.826	-0.042	(0)
CuCl2	6.310e-19	6.311e-19	-18.200	-18.200	0.000	31.02
CuCl3-	9.852e-26	9.616e-26	-25.006	-25.017	-0.011	(0)
CuCl4-2	2.279e-32	2.070e-32	-31.642	-31.684	-0.042	(0)
Fe(2)	4.174e-11					
Fe+2	3.583e-11	3.256e-11	-10.446	-10.487	-0.042	-22.17
FeOH+	4.199e-12	4.099e-12	-11.377	-11.387	-0.010	(0)
FeCO3	1.175e-12	1.175e-12	-11.930	-11.930	0.000	(0)
FeHCO3+	2.688e-13	2.624e-13	-12.571	-12.581	-0.011	(0)
FeSO4	2.585e-13	2.585e-13	-12.588	-12.588	0.000	18.97
Fe(OH)2	1.389e-14	1.389e-14	-13.857	-13.857	0.000	(0)
FeCl+	1.978e-15	1.930e-15	-14.704	-14.714	-0.011	(0)
Fe(OH)3-	2.104e-16	2.054e-16	-15.677	-15.687	-0.010	(0)
FeHSO4+	4.373e-21	4.268e-21	-20.359	-20.370	-0.011	(0)
Fe(3)	7.520e-07					
Fe(OH)3	5.403e-07	5.403e-07	-6.267	-6.267	0.000	(0)
Fe(OH)4-	2.010e-07	1.962e-07	-6.697	-6.707	-0.010	(0)
Fe(OH)2+	1.079e-08	1.054e-08	-7.967	-7.977	-0.010	(0)
FeOH+2	8.800e-14	7.993e-14	-13.056	-13.097	-0.042	(0)
Fe+3	3.840e-20	3.109e-20	-19.416	-19.507	-0.092	(0)
FeSO4+	1.559e-20	1.522e-20	-19.807	-19.818	-0.010	(0)
FeCl+2	4.441e-23	4.033e-23	-22.353	-22.394	-0.042	(0)
Fe(SO4)2-	1.523e-23	1.487e-23	-22.817	-22.828	-0.011	(0)
Fe2(OH)2+4	2.533e-25	1.719e-25	-24.596	-24.765	-0.168	(0)
FeCl2+	7.925e-27	7.737e-27	-26.101	-26.111	-0.010	(0)
FeHSO4+2	1.128e-28	1.024e-28	-27.948	-27.990	-0.042	(0)
Fe3(OH)4+5	6.936e-31	3.785e-31	-30.159	-30.422	-0.263	(0)
FeCl3	3.323e-32	3.323e-32	-31.479	-31.478	0.000	(0)
H(0)	8.933e-29					
H2	4.466e-29	4.467e-29	-28.350	-28.350	0.000	28.61
K	1.407e-05					
K+	1.406e-05	1.372e-05	-4.852	-4.863	-0.011	9.00
KSO4-	4.410e-09	4.305e-09	-8.356	-8.366	-0.010	34.09
Mg	1.892e-05					
Mg+2	1.868e-05	1.697e-05	-4.729	-4.770	-0.042	-21.86
MgSO4	1.776e-07	1.776e-07	-6.750	-6.750	0.000	5.84
MgOH+	2.512e-08	2.453e-08	-7.600	-7.610	-0.010	(0)
MgCO3	2.437e-08	2.437e-08	-7.613	-7.613	0.000	-17.09
MgHCO3+	1.640e-08	1.600e-08	-7.785	-7.796	-0.011	5.47
Mn(2)	1.820e-07					
Mn+2	1.608e-07	1.461e-07	-6.794	-6.835	-0.042	-21.34
MnCO3	1.746e-08	1.746e-08	-7.758	-7.758	0.000	(0)
MnOH+	1.532e-09	1.495e-09	-8.815	-8.825	-0.010	(0)
MnSO4	1.160e-09	1.160e-09	-8.936	-8.936	0.000	22.54

MnHCO3+	1.075e-09	1.049e-09	-8.969	-8.979	-0.010	(0)
MnCl+	2.619e-11	2.556e-11	-10.582	-10.592	-0.010	-3.10
MnCl2	4.792e-16	4.793e-16	-15.319	-15.319	0.000	85.89
Mn(OH)3-	1.497e-16	1.461e-16	-15.825	-15.835	-0.010	(0)
MnCl3-	5.807e-21	5.669e-21	-20.236	-20.246	-0.010	43.34
Mn(3)	5.576e-29					
Mn+3	5.576e-29	4.515e-29	-28.254	-28.345	-0.092	(0)
Na	5.002e-05					
Na+	5.001e-05	4.882e-05	-4.301	-4.311	-0.010	-1.49
NaSO4-	1.119e-08	1.092e-08	-7.951	-7.962	-0.010	13.65
NaHCO3	2.212e-09	2.212e-09	-8.655	-8.655	0.000	1.80
NaCO3-	1.401e-09	1.368e-09	-8.853	-8.864	-0.011	-1.04
NaOH	1.967e-20	1.967e-20	-19.706	-19.706	0.000	(0)
O(0)	3.125e-04					
O2	1.563e-04	1.563e-04	-3.806	-3.806	0.000	30.40
Pb	1.931e-07					
PbCO3	1.379e-07	1.379e-07	-6.860	-6.860	0.000	(0)
PbOH+	4.194e-08	4.094e-08	-7.377	-7.388	-0.011	(0)
Pb(OH)2	6.340e-09	6.341e-09	-8.198	-8.198	0.000	(0)
Pb+2	5.811e-09	5.274e-09	-8.236	-8.278	-0.042	-15.58
Pb(CO3)2-2	5.742e-10	5.212e-10	-9.241	-9.283	-0.042	(0)
PbHCO3+	3.459e-10	3.376e-10	-9.461	-9.472	-0.011	(0)
PbSO4	1.324e-10	1.324e-10	-9.878	-9.878	0.000	(0)
Pb(OH)3-	2.969e-11	2.898e-11	-10.527	-10.538	-0.011	(0)
PbCl+	9.239e-12	9.017e-12	-11.034	-11.045	-0.011	7.94
Pb(SO4)2-2	3.418e-14	3.103e-14	-13.466	-13.508	-0.042	(0)
Pb(OH)4-2	2.912e-14	2.643e-14	-13.536	-13.578	-0.042	(0)
Pb2OH+3	6.011e-15	4.834e-15	-14.221	-14.316	-0.095	(0)
Pb3(OH)4+2	5.352e-15	4.857e-15	-14.272	-14.314	-0.042	(0)
PbCl2	6.137e-16	6.138e-16	-15.212	-15.212	0.000	34.97
PbCl3-	2.145e-20	2.094e-20	-19.669	-19.679	-0.011	65.94
PbCl4-2	4.742e-25	4.304e-25	-24.324	-24.366	-0.042	101.31
S(6)	5.007e-05					
SO4-2	4.916e-05	4.465e-05	-4.308	-4.350	-0.042	14.47
CaSO4	7.069e-07	7.070e-07	-6.151	-6.151	0.000	7.50
MgSO4	1.776e-07	1.776e-07	-6.750	-6.750	0.000	5.84
NaSO4-	1.119e-08	1.092e-08	-7.951	-7.962	-0.010	13.65
BaSO4	1.013e-08	1.013e-08	-7.994	-7.994	0.000	(0)
KSO4-	4.410e-09	4.305e-09	-8.356	-8.366	-0.010	34.09
MnSO4	1.160e-09	1.160e-09	-8.936	-8.936	0.000	22.54
CdSO4	6.925e-10	6.925e-10	-9.160	-9.160	0.000	78.05
PbSO4	1.324e-10	1.324e-10	-9.878	-9.878	0.000	(0)
HSO4-	1.117e-11	1.090e-11	-10.952	-10.962	-0.011	40.27
CuSO4	2.157e-12	2.158e-12	-11.666	-11.666	0.000	13.09
Cd(SO4)2-2	3.735e-13	3.390e-13	-12.428	-12.470	-0.042	-105.68
FeSO4	2.585e-13	2.585e-13	-12.588	-12.588	0.000	18.97
Pb(SO4)2-2	3.418e-14	3.103e-14	-13.466	-13.508	-0.042	(0)
CaHSO4+	1.196e-14	1.167e-14	-13.922	-13.933	-0.011	(0)
AlSO4+	7.410e-18	7.233e-18	-17.130	-17.141	-0.010	(0)
FeSO4+	1.559e-20	1.522e-20	-19.807	-19.818	-0.010	(0)
Al(SO4)2-	1.046e-20	1.021e-20	-19.980	-19.991	-0.010	(0)
FeHSO4+	4.373e-21	4.268e-21	-20.359	-20.370	-0.011	(0)
Fe(SO4)2-	1.523e-23	1.487e-23	-22.817	-22.828	-0.011	(0)
AlHSO4+2	1.775e-27	1.611e-27	-26.751	-26.793	-0.042	(0)
FeHSO4+2	1.128e-28	1.024e-28	-27.948	-27.990	-0.042	(0)
Si	4.644e-05					
H4SiO4	4.380e-05	4.381e-05	-4.359	-4.358	0.000	52.08
H3SiO4-	2.635e-06	2.571e-06	-5.579	-5.590	-0.011	27.96
H2SiO4-2	7.665e-11	6.964e-11	-10.115	-10.157	-0.042	(0)

-------------------------------Saturation indices--------------------------------

Phase	SI**	log IAP	log K(298 K, 1 atm)	
Al(OH)3(a)	-1.29	9.51	10.80	Al(OH)3
Albite	-3.94	-21.94	-18.00	NaAlSi3O8
Alunite	-9.43	-10.83	-1.40	KAl3(SO4)2(OH)6
Anglesite	-4.84	-12.63	-7.79	PbSO4

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  Anhydrite          -4.12     -8.40   -4.28  CaSO4
  Anorthite          -2.16    -21.88  -19.71  CaAl2Si2O8
  Aragonite          -1.54     -9.87   -8.34  CaCO3
  Barite             -0.72    -10.69   -9.97  BaSO4
  Ca-Montmorillonite  0.55    -44.48  -45.03  Ca0.165Al2.33Si3.67O10(OH)2
  Calcite            -1.39     -9.87   -8.48  CaCO3
  Cd(OH)2            -3.72      9.93   13.65  Cd(OH)2
  CdSiO3             -3.49      5.57    9.06  CdSiO3
  CdSO4             -11.52    -11.62   -0.10  CdSO4
  Cerrusite          -0.97    -14.10  -13.13  PbCO3
  Chalcedony         -0.81     -4.36   -3.55  SiO2
  Chlorite(14A)      -0.29     68.09   68.38  Mg5Al2Si3O10(OH)8
  Chrysotile         -3.63     28.57   32.20  Mg3Si2O5(OH)4
  CO2(g)             -4.88     -6.34   -1.46  CO2
  Dolomite           -3.38    -20.47  -17.09  CaMg(CO3)2
  Fe(OH)3(a)          1.40      6.29    4.89  Fe(OH)3
  Gibbsite            1.40      9.51    8.11  Al(OH)3
  Goethite            7.29      6.29   -1.00  FeOOH
  Gypsum             -3.82     -8.40   -4.58  CaSO4:2H2O
  H2(g)             -25.25    -28.35   -3.10  H2
  H2O(g)             -1.50     -0.00    1.50  H2O
  Halite            -10.25     -8.68    1.57  NaCl
  Hausmannite        -4.74     56.29   61.03  Mn3O4
  Hematite           16.59     12.59   -4.01  Fe2O3
  Illite              0.10    -40.16  -40.27  K0.6Mg0.25Al2.3Si3.5O10(OH)2
  Jarosite-K        -11.27    -20.48   -9.21  KFe3(SO4)2(OH)6
  K-feldspar         -1.92    -22.49  -20.57  KAlSi3O8
  K-mica              6.49     19.19   12.70  KAl3Si3O10(OH)2
  Kaolinite           2.87     10.30    7.43  Al2Si2O5(OH)4
  Manganite          -2.38     22.96   25.34  MnOOH
  Melanterite       -12.63    -14.84   -2.21  FeSO4:7H2O
  O2(g)              -0.91     -3.81   -2.89  O2
  Otavite            -0.99    -13.09  -12.10  CdCO3
  Pb(OH)2             0.77      8.92    8.15  Pb(OH)2
  Pyrochroite        -4.84     10.36   15.20  Mn(OH)2
  Pyrolusite         -5.82     35.56   41.38  MnO2:H2O
  Quartz             -0.38     -4.36   -3.98  SiO2
  Rhodochrosite      -1.53    -12.66  -11.13  MnCO3
  Sepiolite          -3.98     11.78   15.76  Mg2Si3O7.5OH:3H2O
  Sepiolite(d)       -6.88     11.78   18.66  Mg2Si3O7.5OH:3H2O
  Siderite           -5.42    -16.31  -10.89  FeCO3
  SiO2(a)            -1.65     -4.36   -2.71  SiO2
  Sylvite           -10.13     -9.23    0.90  KCl
  Talc               -1.54     19.86   21.40  Mg3Si4O10(OH)2
  Witherite          -3.60    -12.17   -8.56  BaCO3

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
  For ideal gases, phi = 1.

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End of simulation.
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Reading input data for simulation 3.
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      TITLE Aqua Mix part III: mix 90% soln 1, 10% soln 2.
      MIX 1
              1      0.90
              2      0.10
      SAVE solution   3
      END
-----
TITLE
-----

 Aqua Mix part III: mix 90% soln 1, 10% soln 2.
```

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----------------------------------------
Beginning of batch-reaction calculations.
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Reaction step 1.

Using mix 1.

Mixture 1.

        9.000e-01 Solution 1  MW-4
        1.000e-01 Solution 2  DI Extraction

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

      Elements           Molality       Moles

      Al                4.522e-06   4.522e-06
      Ba                5.098e-07   5.098e-07
      C                 2.005e-03   2.005e-03
      Ca                9.007e-04   9.007e-04
      Cd                6.228e-09   6.228e-09
      Cl                3.701e-04   3.701e-04
      Cu                5.037e-07   5.037e-07
      Fe                7.521e-08   7.521e-08
      K                 8.820e-05   8.820e-05
      Mg                1.519e-04   1.519e-04
      Mn                1.820e-08   1.820e-08
      Na                1.117e-03   1.117e-03
      Pb                1.323e-07   1.323e-07
      S                 3.123e-04   3.123e-04
      Si                1.876e-04   1.876e-04

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

                                     pH  =   7.869      Charge balance
                                     pe  =  13.591      Adjusted to redox equilibrium
       Specific Conductance (µS/cm, 15°C)  = 246
                            Density (g/cm³)  =   0.99930
                                 Volume (L)  =   1.00096
                          Activity of water  =   1.000
                             Ionic strength  =   4.345e-03
                         Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   1.974e-03
                        Total CO2 (mol/kg)  =   2.005e-03
                          Temperature (°C)  =  15.01
                   Electrical balance (eq)  =   3.574e-04
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   5.86
                                Iterations  =  18
                                   Total H  = 1.110151e+02
                                   Total O  = 5.551462e+01

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

                                                 Log       Log       Log    mole V
   Species          Molality    Activity  Molality  Activity     Gamma   cm³/mol

   OH-             3.607e-07   3.361e-07    -6.443    -6.474    -0.031     -4.59
   H+              1.440e-08   1.351e-08    -7.842    -7.869    -0.028      0.00
   H2O             5.551e+01   9.999e-01     1.744    -0.000     0.000     18.03
Al            4.522e-06
   Al(OH)4-        4.482e-06   4.181e-06    -5.349    -5.379    -0.030       (0)
   Al(OH)3         3.330e-08   3.333e-08    -7.478    -7.477     0.000       (0)
   Al(OH)2+        7.189e-09   6.715e-09    -8.143    -8.173    -0.030       (0)
   AlOH+2          3.840e-11   2.923e-11   -10.416   -10.534    -0.118    -27.29
   Al+3            1.371e-13   7.722e-14   -12.863   -13.112    -0.249    -41.39
   AlSO4+          4.929e-14   4.599e-14   -13.307   -13.337    -0.030       (0)
```

Al(SO4)2-	3.199e-16	2.985e-16	-15.495	-15.525	-0.030	(0)
AlHSO4+2	6.762e-23	5.112e-23	-22.170	-22.291	-0.121	(0)
Ba	5.098e-07					
Ba+2	4.663e-07	3.528e-07	-6.331	-6.452	-0.121	-13.30
BaSO4	3.804e-08	3.808e-08	-7.420	-7.419	0.000	(0)
BaHCO3+	4.733e-09	4.413e-09	-8.325	-8.355	-0.030	(0)
BaCO3	7.352e-10	7.359e-10	-9.134	-9.133	0.000	-10.81
BaOH+	9.479e-13	8.849e-13	-12.023	-12.053	-0.030	(0)
C(-4)	0.000e+00					
CH4	0.000e+00	0.000e+00	-150.105	-150.105	0.000	32.22
C(4)	2.005e-03					
HCO3-	1.913e-03	1.787e-03	-2.718	-2.748	-0.030	23.81
CO2	6.325e-05	6.332e-05	-4.199	-4.198	0.000	31.86
CaHCO3+	1.320e-05	1.234e-05	-4.879	-4.909	-0.029	9.25
CO3-2	6.482e-06	4.934e-06	-5.188	-5.307	-0.118	-6.30
CaCO3	4.611e-06	4.616e-06	-5.336	-5.336	0.000	-14.63
MgHCO3+	2.395e-06	2.233e-06	-5.621	-5.651	-0.030	5.16
NaHCO3	1.107e-06	1.108e-06	-5.956	-5.955	0.000	1.80
MgCO3	4.457e-07	4.461e-07	-6.351	-6.351	0.000	-17.08
PbCO3	1.237e-07	1.238e-07	-6.908	-6.907	0.000	(0)
CuCO3	9.250e-08	9.259e-08	-7.034	-7.033	0.000	(0)
NaCO3-	6.086e-08	5.675e-08	-7.216	-7.246	-0.030	-2.15
BaHCO3+	4.733e-09	4.413e-09	-8.325	-8.355	-0.030	(0)
MnCO3	3.740e-09	3.744e-09	-8.427	-8.427	0.000	(0)
CuHCO3+	3.356e-09	3.130e-09	-8.474	-8.505	-0.030	(0)
PbHCO3+	2.198e-09	2.049e-09	-8.658	-8.688	-0.030	(0)
Pb(CO3)2-2	2.029e-09	1.534e-09	-8.693	-8.814	-0.121	(0)
MnHCO3+	1.630e-09	1.521e-09	-8.788	-8.818	-0.030	(0)
Cu(CO3)2-2	7.608e-10	5.751e-10	-9.119	-9.240	-0.121	(0)
BaCO3	7.352e-10	7.359e-10	-9.134	-9.133	0.000	-10.81
CdHCO3+	2.544e-10	2.372e-10	-9.595	-9.625	-0.030	(0)
CdCO3	1.643e-11	1.645e-11	-10.784	-10.784	0.000	(0)
Cd(CO3)2-2	3.395e-13	2.567e-13	-12.469	-12.591	-0.121	(0)
FeHCO3+	2.132e-19	1.988e-19	-18.671	-18.702	-0.030	(0)
FeCO3	1.315e-19	1.317e-19	-18.881	-18.881	0.000	(0)
Ca	9.007e-04					
Ca+2	8.597e-04	6.541e-04	-3.066	-3.184	-0.119	-18.20
CaSO4	2.316e-05	2.318e-05	-4.635	-4.635	0.000	7.06
CaHCO3+	1.320e-05	1.234e-05	-4.879	-4.909	-0.029	9.25
CaCO3	4.611e-06	4.616e-06	-5.336	-5.336	0.000	-14.63
CaOH+	8.618e-09	8.036e-09	-8.065	-8.095	-0.030	(0)
CaHSO4+	1.936e-12	1.805e-12	-11.713	-11.743	-0.030	(0)
Cd	6.228e-09					
Cd+2	5.552e-09	4.197e-09	-8.256	-8.377	-0.121	-19.23
CdHCO3+	2.544e-10	2.372e-10	-9.595	-9.625	-0.030	(0)
CdSO4	2.444e-10	2.447e-10	-9.612	-9.611	0.000	83.78
CdCl+	1.432e-10	1.335e-10	-9.844	-9.874	-0.030	2.88
CdCO3	1.643e-11	1.645e-11	-10.784	-10.784	0.000	(0)
CdOH+	1.288e-11	1.201e-11	-10.890	-10.921	-0.030	(0)
CdOHCl	3.272e-12	3.276e-12	-11.485	-11.485	0.000	(0)
Cd(SO4)2-2	8.141e-13	6.154e-13	-12.089	-12.211	-0.121	-113.36
Cd(CO3)2-2	3.395e-13	2.567e-13	-12.469	-12.591	-0.121	(0)
CdCl2	1.847e-13	1.848e-13	-12.734	-12.733	0.000	23.14
Cd(OH)2	1.026e-13	1.027e-13	-12.989	-12.988	0.000	(0)
CdCl3-	3.692e-17	3.442e-17	-16.433	-16.463	-0.030	77.65
Cd(OH)3-	9.149e-19	8.531e-19	-18.039	-18.069	-0.030	(0)
Cd2OH+3	5.268e-19	2.807e-19	-18.278	-18.552	-0.273	(0)
Cd(OH)4-2	7.445e-25	5.628e-25	-24.128	-24.250	-0.121	(0)
CdHS+	0.000e+00	0.000e+00	-146.216	-146.246	-0.030	(0)
Cd(HS)2	0.000e+00	0.000e+00	-287.926	-287.925	0.000	(0)
Cd(HS)3-	0.000e+00	0.000e+00	-433.754	-433.784	-0.030	(0)
Cd(HS)4-2	0.000e+00	0.000e+00	-579.512	-579.633	-0.121	(0)
Cl	3.701e-04					
Cl-	3.701e-04	3.449e-04	-3.432	-3.462	-0.031	17.71
CdCl+	1.432e-10	1.335e-10	-9.844	-9.874	-0.030	2.88
PbCl+	1.645e-11	1.534e-11	-10.784	-10.814	-0.030	7.54
MnCl+	1.438e-11	1.342e-11	-10.842	-10.872	-0.030	-6.07
CdOHCl	3.272e-12	3.276e-12	-11.485	-11.485	0.000	(0)

CuCl+	2.097e-12	1.955e-12	-11.678	-11.709	-0.030	3.67
CdCl2	1.847e-13	1.848e-13	-12.734	-12.733	0.000	23.14
PbCl2	1.016e-14	1.017e-14	-13.993	-13.993	0.000	34.03
MnCl2	2.018e-15	2.021e-15	-14.695	-14.695	0.000	100.15
CuCl2	3.235e-16	3.238e-16	-15.490	-15.490	0.000	17.55
CdCl3-	3.692e-17	3.442e-17	-16.433	-16.463	-0.030	77.65
PbCl3-	2.803e-18	2.614e-18	-17.552	-17.583	-0.030	64.55
MnCl3-	2.056e-19	1.919e-19	-18.687	-18.717	-0.030	43.74
FeCl+2	2.322e-20	1.764e-20	-19.634	-19.754	-0.119	(0)
CuCl2-	1.766e-21	1.647e-21	-20.753	-20.783	-0.030	(0)
FeCl+	5.679e-22	5.296e-22	-21.246	-21.276	-0.030	(0)
PbCl4-2	5.271e-22	3.985e-22	-21.278	-21.400	-0.121	99.54
CuCl3-	3.539e-22	3.300e-22	-21.451	-21.482	-0.030	(0)
FeCl2+	4.038e-23	3.770e-23	-22.394	-22.424	-0.030	(0)
CuCl3-2	1.139e-24	8.651e-25	-23.944	-24.063	-0.119	(0)
FeCl3	1.299e-27	1.300e-27	-26.886	-26.886	0.000	(0)
CuCl4-2	5.910e-28	4.490e-28	-27.228	-27.348	-0.119	(0)
Cu(1)	4.769e-20					
Cu+	4.592e-20	4.272e-20	-19.338	-19.369	-0.031	(0)
CuCl2-	1.766e-21	1.647e-21	-20.753	-20.783	-0.030	(0)
CuCl3-2	1.139e-24	8.651e-25	-23.944	-24.063	-0.119	(0)
Cu(2)	5.037e-07					
Cu(OH)2	3.996e-07	4.000e-07	-6.398	-6.398	0.000	(0)
CuCO3	9.250e-08	9.259e-08	-7.034	-7.033	0.000	(0)
Cu+2	4.576e-09	3.494e-09	-8.340	-8.457	-0.117	-26.45
CuHCO3+	3.356e-09	3.130e-09	-8.474	-8.505	-0.030	(0)
CuOH+	2.774e-09	2.586e-09	-8.557	-8.587	-0.030	(0)
Cu(CO3)2-2	7.608e-10	5.751e-10	-9.119	-9.240	-0.121	(0)
CuSO4	1.429e-10	1.430e-10	-9.845	-9.845	0.000	11.64
CuCl+	2.097e-12	1.955e-12	-11.678	-11.709	-0.030	3.67
Cu(OH)3-	1.913e-12	1.784e-12	-11.718	-11.749	-0.030	(0)
Cu2(OH)2+2	1.387e-12	1.049e-12	-11.858	-11.979	-0.121	(0)
CuCl2	3.235e-16	3.238e-16	-15.490	-15.490	0.000	17.55
Cu(OH)4-2	3.485e-17	2.635e-17	-16.458	-16.579	-0.121	(0)
CuCl3-	3.539e-22	3.300e-22	-21.451	-21.482	-0.030	(0)
CuCl4-2	5.910e-28	4.490e-28	-27.228	-27.348	-0.119	(0)
Cu(HS)3-	0.000e+00	0.000e+00	-426.643	-426.674	-0.030	(0)
Fe(2)	1.850e-18					
Fe+2	1.457e-18	1.112e-18	-17.837	-17.954	-0.117	-22.75
FeHCO3+	2.132e-19	1.988e-19	-18.671	-18.702	-0.030	(0)
FeCO3	1.315e-19	1.317e-19	-18.881	-18.881	0.000	(0)
FeSO4	3.522e-20	3.526e-20	-19.453	-19.453	0.000	31.15
FeOH+	1.288e-20	1.203e-20	-19.890	-19.920	-0.030	(0)
FeCl+	5.679e-22	5.296e-22	-21.246	-21.276	-0.030	(0)
Fe(OH)2	3.081e-24	3.084e-24	-23.511	-23.511	0.000	(0)
Fe(OH)3-	8.207e-27	7.662e-27	-26.086	-26.116	-0.030	(0)
FeHSO4+	3.292e-27	3.070e-27	-26.483	-26.513	-0.030	(0)
Fe(HS)2	0.000e+00	0.000e+00	-305.082	-305.082	0.000	(0)
Fe(HS)3-	0.000e+00	0.000e+00	-451.054	-451.084	-0.030	(0)
Fe(3)	7.521e-08					
Fe(OH)3	6.144e-08	6.150e-08	-7.212	-7.211	0.000	(0)
Fe(OH)2+	1.083e-08	1.012e-08	-7.965	-7.995	-0.030	(0)
Fe(OH)4-	2.934e-09	2.740e-09	-8.533	-8.562	-0.030	(0)
FeOH+2	8.045e-13	6.111e-13	-12.094	-12.214	-0.119	(0)
FeSO4+	4.727e-18	4.413e-18	-17.325	-17.355	-0.030	(0)
Fe+3	4.172e-18	2.350e-18	-17.380	-17.629	-0.249	(0)
FeCl+2	2.322e-20	1.764e-20	-19.634	-19.754	-0.119	(0)
Fe(SO4)2-	2.141e-20	1.997e-20	-19.669	-19.700	-0.030	(0)
Fe2(OH)2+4	4.717e-23	1.541e-23	-22.326	-22.812	-0.486	(0)
FeCl2+	4.038e-23	3.770e-23	-22.394	-22.424	-0.030	(0)
FeHSO4+2	2.155e-25	1.629e-25	-24.667	-24.788	-0.121	(0)
FeCl3	1.299e-27	1.300e-27	-26.886	-26.886	0.000	(0)
Fe3(OH)4+5	4.857e-28	8.455e-29	-27.314	-28.073	-0.759	(0)
H(0)	0.000e+00					
H2	0.000e+00	0.000e+00	-46.026	-46.026	0.000	28.62
K	8.820e-05					
K+	8.809e-05	8.208e-05	-4.055	-4.086	-0.031	8.66
KSO4-	1.110e-07	1.037e-07	-6.955	-6.984	-0.030	33.80

Mg	1.519e-04					
Mg+2	1.447e-04	1.105e-04	-3.839	-3.957	-0.117	-21.34
MgSO4	4.268e-06	4.272e-06	-5.370	-5.369	0.000	5.40
MgHCO3+	2.395e-06	2.233e-06	-5.621	-5.651	-0.030	5.16
MgCO3	4.457e-07	4.461e-07	-6.351	-6.351	0.000	-17.08
MgOH+	1.248e-08	1.167e-08	-7.904	-7.933	-0.029	(0)
Mn(2)	1.820e-08					
Mn+2	1.251e-08	9.553e-09	-7.903	-8.020	-0.117	-20.59
MnCO3	3.740e-09	3.744e-09	-8.427	-8.427	0.000	(0)
MnHCO3+	1.630e-09	1.521e-09	-8.788	-8.818	-0.030	(0)
MnSO4	3.000e-10	3.003e-10	-9.523	-9.522	0.000	27.68
MnCl+	1.438e-11	1.342e-11	-10.842	-10.872	-0.030	-6.07
MnOH+	8.383e-12	7.826e-12	-11.077	-11.106	-0.030	(0)
MnCl2	2.018e-15	2.021e-15	-14.695	-14.695	0.000	100.15
MnCl3-	2.056e-19	1.919e-19	-18.687	-18.717	-0.030	43.74
Mn(OH)3-	6.577e-20	6.140e-20	-19.182	-19.212	-0.030	(0)
Mn(3)	4.514e-21					
Mn+3	4.514e-21	2.543e-21	-20.345	-20.595	-0.249	(0)
Na	1.117e-03					
Na+	1.115e-03	1.040e-03	-2.953	-2.983	-0.030	-2.04
NaSO4-	1.126e-06	1.051e-06	-5.949	-5.978	-0.030	14.22
NaHCO3	1.107e-06	1.108e-06	-5.956	-5.955	0.000	1.80
NaCO3-	6.086e-08	5.675e-08	-7.216	-7.246	-0.030	-2.15
NaOH	3.493e-20	3.496e-20	-19.457	-19.456	0.000	(0)
O(0)	4.324e-04					
O2	2.162e-04	2.164e-04	-3.665	-3.665	0.000	29.51
Pb	1.323e-07					
PbCO3	1.237e-07	1.238e-07	-6.908	-6.907	0.000	(0)
PbOH+	2.234e-09	2.083e-09	-8.651	-8.681	-0.030	(0)
PbHCO3+	2.198e-09	2.049e-09	-8.658	-8.688	-0.030	(0)
Pb(CO3)2-2	2.029e-09	1.534e-09	-8.693	-8.814	-0.121	(0)
Pb+2	1.909e-09	1.444e-09	-8.719	-8.841	-0.121	-15.35
PbSO4	1.746e-10	1.748e-10	-9.758	-9.757	0.000	(0)
Pb(OH)2	5.994e-11	6.000e-11	-10.222	-10.222	0.000	(0)
PbCl+	1.645e-11	1.534e-11	-10.784	-10.814	-0.030	7.54
Pb(SO4)2-2	2.613e-13	1.975e-13	-12.583	-12.704	-0.121	(0)
Pb(OH)3-	5.468e-14	5.099e-14	-13.262	-13.293	-0.030	(0)
PbCl2	1.016e-14	1.017e-14	-13.993	-13.993	0.000	34.03
Pb2OH+3	1.263e-16	6.733e-17	-15.898	-16.172	-0.273	(0)
Pb(OH)4-2	1.144e-17	8.646e-18	-16.942	-17.063	-0.121	(0)
PbCl3-	2.803e-18	2.614e-18	-17.552	-17.583	-0.030	64.55
Pb3(OH)4+2	3.340e-20	2.525e-20	-19.476	-19.598	-0.121	(0)
PbCl4-2	5.271e-22	3.985e-22	-21.278	-21.400	-0.121	99.54
Pb(HS)2	0.000e+00	0.000e+00	-289.649	-289.649	0.000	(0)
Pb(HS)3-	0.000e+00	0.000e+00	-436.357	-436.388	-0.030	(0)
S(-2)	0.000e+00					
CdHS+	0.000e+00	0.000e+00	-146.216	-146.246	-0.030	(0)
HS-	0.000e+00	0.000e+00	-148.008	-148.039	-0.031	20.05
H2S	0.000e+00	0.000e+00	-148.824	-148.824	0.000	37.12
S-2	0.000e+00	0.000e+00	-153.276	-153.395	-0.119	(0)
Cd(HS)2	0.000e+00	0.000e+00	-287.926	-287.925	0.000	(0)
Pb(HS)2	0.000e+00	0.000e+00	-289.649	-289.649	0.000	(0)
Fe(HS)2	0.000e+00	0.000e+00	-305.082	-305.082	0.000	(0)
Cu(HS)3-	0.000e+00	0.000e+00	-426.643	-426.674	-0.030	(0)
Cd(HS)3-	0.000e+00	0.000e+00	-433.754	-433.784	-0.030	(0)
Pb(HS)3-	0.000e+00	0.000e+00	-436.357	-436.388	-0.030	(0)
Fe(HS)3-	0.000e+00	0.000e+00	-451.054	-451.084	-0.030	(0)
Cd(HS)4-2	0.000e+00	0.000e+00	-579.512	-579.633	-0.121	(0)
S(6)	3.123e-04					
SO4-2	2.836e-04	2.153e-04	-3.547	-3.667	-0.120	13.01
CaSO4	2.316e-05	2.318e-05	-4.635	-4.635	0.000	7.06
MgSO4	4.268e-06	4.272e-06	-5.370	-5.369	0.000	5.40
NaSO4-	1.126e-06	1.051e-06	-5.949	-5.978	-0.030	14.22
KSO4-	1.110e-07	1.037e-07	-6.955	-6.984	-0.030	33.80
BaSO4	3.804e-08	3.808e-08	-7.420	-7.419	0.000	(0)
MnSO4	3.000e-10	3.003e-10	-9.523	-9.522	0.000	27.68
HSO4-	2.462e-10	2.295e-10	-9.609	-9.639	-0.030	39.48
CdSO4	2.444e-10	2.447e-10	-9.612	-9.611	0.000	83.78

PbSO4	1.746e-10	1.748e-10	-9.758	-9.757	0.000	(0)
CuSO4	1.429e-10	1.430e-10	-9.845	-9.845	0.000	11.64
CaHSO4+	1.936e-12	1.805e-12	-11.713	-11.743	-0.030	(0)
Cd(SO4)2-2	8.141e-13	6.154e-13	-12.089	-12.211	-0.121	-113.36
Pb(SO4)2-2	2.613e-13	1.975e-13	-12.583	-12.704	-0.121	(0)
AlSO4+	4.929e-14	4.599e-14	-13.307	-13.337	-0.030	(0)
Al(SO4)2-	3.199e-16	2.985e-16	-15.495	-15.525	-0.030	(0)
FeSO4+	4.727e-18	4.413e-18	-17.325	-17.355	-0.030	(0)
FeSO4	3.522e-20	3.526e-20	-19.453	-19.453	0.000	31.15
Fe(SO4)2-	2.141e-20	1.997e-20	-19.669	-19.700	-0.030	(0)
AlHSO4+2	6.762e-23	5.112e-23	-22.170	-22.291	-0.121	(0)
FeHSO4+2	2.155e-25	1.629e-25	-24.667	-24.788	-0.121	(0)
FeHSO4+	3.292e-27	3.070e-27	-26.483	-26.513	-0.030	(0)
Si	1.876e-04					
H4SiO4	1.861e-04	1.863e-04	-3.730	-3.730	0.000	53.05
H3SiO4-	1.505e-06	1.403e-06	-5.823	-5.853	-0.030	27.67
H2SiO4-2	4.651e-12	3.541e-12	-11.332	-11.451	-0.118	(0)

----------Saturation indices----------

Phase	SI**	log IAP	log K(288 K, 1 atm)	
Al(OH)3(a)	-0.98	10.50	11.47	Al(OH)3
Albite	-0.89	-19.55	-18.66	NaAlSi3O8
Alunite	-3.42	-3.54	-0.12	KAl3(SO4)2(OH)6
Anglesite	-4.66	-12.51	-7.84	PbSO4
Anhydrite	-2.68	-6.85	-4.17	CaSO4
Anorthite	-1.39	-21.40	-20.01	CaAl2Si2O8
Aragonite	-0.21	-8.49	-8.28	CaCO3
Barite	0.02	-10.12	-10.14	BaSO4
Ca-Montmorillonite	4.03	-42.48	-46.51	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	-0.06	-8.49	-8.43	CaCO3
Cd(OH)2	-6.29	7.36	13.65	Cd(OH)2
CdSiO3	-5.85	3.63	9.48	CdSiO3
CdSO4	-12.32	-12.04	0.27	CdSO4
Cerrusite	-0.89	-14.15	-13.25	PbCO3
CH4(g)	-147.35	-150.10	-2.76	CH4
Chalcedony	-0.06	-3.73	-3.67	SiO2
Chlorite(14A)	-3.52	68.71	72.23	Mg5Al2Si3O10(OH)8
Chrysotile	-5.59	27.89	33.48	Mg3Si2O5(OH)4
CO2(g)	-2.86	-4.20	-1.34	CO2
Dolomite	-0.90	-17.75	-16.85	CaMg(CO3)2
Fe(OH)3(a)	1.09	5.98	4.89	Fe(OH)3
FeS(ppt)	-154.21	-158.12	-3.92	FeS
Gibbsite	1.81	10.50	8.69	Al(OH)3
Goethite	6.61	5.98	-0.63	FeOOH
Gypsum	-2.27	-6.85	-4.58	CaSO4:2H2O
H2(g)	-42.95	-46.03	-3.07	H2
H2O(g)	-1.77	-0.00	1.77	H2O
H2S(g)	-147.89	-155.91	-8.02	H2S
Halite	-8.01	-6.45	1.56	NaCl
Hausmannite	2.49	66.08	63.59	Mn3O4
Hematite	15.18	11.96	-3.22	Fe2O3
Illite	3.35	-38.31	-41.66	K0.6Mg0.25Al2.3Si3.5O10(OH)2
Jarosite-K	-8.68	-17.09	-8.42	KFe3(SO4)2(OH)6
K-feldspar	0.70	-20.65	-21.36	KAlSi3O8
K-mica	9.87	24.08	14.21	KAl3Si3O10(OH)2
Kaolinite	5.20	13.53	8.33	Al2Si2O5(OH)4
Mackinawite	-153.48	-158.12	-4.65	FeS
Manganite	3.84	29.18	25.34	MnOOH
Melanterite	-19.28	-21.62	-2.34	FeSO4:7H2O
O2(g)	-0.85	-3.66	-2.81	O2
Otavite	-1.58	-13.68	-12.10	CdCO3
Pb(OH)2	-1.61	6.90	8.51	Pb(OH)2
Pyrite	-252.35	-271.11	-18.77	FeS2
Pyrochroite	-7.48	7.72	15.20	Mn(OH)2
Pyrolusite	7.60	50.64	43.03	MnO2:H2O
Quartz	0.40	-3.73	-4.13	SiO2

```
  Rhodochrosite    -2.23    -13.33  -11.09  MnCO3
  Sepiolite        -3.66     12.37   16.03  Mg2Si3O7.5OH:3H2O
  Sepiolite(d)     -6.29     12.37   18.66  Mg2Si3O7.5OH:3H2O
  Siderite        -12.43    -23.26  -10.83  FeCO3
  SiO2(a)          -0.93     -3.73   -2.80  SiO2
  Sulfur         -111.03   -105.90    5.12  S
  Sylvite          -8.40     -7.55    0.85  KCl
  Talc             -2.15     20.43   22.58  Mg3Si4O10(OH)2
  Witherite        -3.16    -11.76   -8.60  BaCO3

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
  For ideal gases, phi = 1.

------------------
End of simulation.
------------------

------------------------------------
Reading input data for simulation 4.
------------------------------------

------------------------------
End of Run after 0.24 Seconds.
------------------------------
```

```
   Input file: E:\Project Stuff\Models\Mixing 50_50.pqi
  Output file: E:\Project Stuff\Models\Mixing 50_50.pqo
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.2.2-10160\database
\phreeqc.dat

------------------
Reading data base.
------------------

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

      DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 3.2.2-10160\database
\phreeqc.dat
      TITLE Water Mixing Scenario Part I
      SOLUTION 1  MW-4
            units   ppm
            temp    13.9
            pH    7.87
            O(0)            7.13
            Ca              39.66
            Mg              4.05
            Na              28.4
            K               3.77
            Ba              0.07
            Be              0
            Cd              0
            Cu              0.03
            Pb              0.026
            Mn              0
            Se              0
            Ni              0.011
            Fe              0
            Al              0.05
            As              0
            Cl              14.4
            Alkalinity      132.4 as HCO3
            S(6)        32.79
            Si    12.21
      SAVE solution 1
      END
-----
TITLE
-----

 Water Mixing Scenario Part I

WARNING: Could not find element in database, As.
      Concentration is set to zero.
WARNING: Could not find element in database, Be.
      Concentration is set to zero.
WARNING: Could not find element in database, Ni.
      Concentration is set to zero.
WARNING: Could not find element in database, Se.
      Concentration is set to zero.
-----------------------------------------
Beginning of initial solution calculations.
-----------------------------------------
```

Initial solution 1. MW-4

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

Elements	Molality	Moles
Al	1.854e-06	1.854e-06
Alkalinity	2.170e-03	2.170e-03
Ba	5.098e-07	5.098e-07
Ca	9.898e-04	9.898e-04
Cl	4.063e-04	4.063e-04
Cu	4.722e-07	4.722e-07
K	9.644e-05	9.644e-05
Mg	1.666e-04	1.666e-04
Na	1.236e-03	1.236e-03
O(0)	4.457e-04	4.457e-04
Pb	1.255e-07	1.255e-07
S(6)	3.414e-04	3.414e-04
Si	2.033e-04	2.033e-04

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

pH	= 7.870
pe	= 4.000
Specific Conductance (µS/cm, 13°C)	= 262
Density (g/cm³)	= 0.99948
Volume (L)	= 1.00080
Activity of water	= 1.000
Ionic strength	= 4.770e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 2.218e-03
Total CO2 (mol/kg)	= 2.218e-03
Temperature (°C)	= 13.90
Electrical balance (eq)	= 3.932e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 5.86
Iterations	= 9
Total H	= 1.110154e+02
Total O	= 5.551543e+01

----------Redox couples----------

Redox couple	pe	Eh (volts)
O(-2)/O(0)	13.6923	0.7798

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	3.297e-07	3.063e-07	-6.482	-6.514	-0.032	-4.67
H+	1.441e-08	1.349e-08	-7.841	-7.870	-0.029	0.00
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.03
Al	1.854e-06					
Al(OH)4-	1.837e-06	1.709e-06	-5.736	-5.767	-0.031	(0)
Al(OH)3	1.370e-08	1.371e-08	-7.863	-7.863	0.000	(0)
Al(OH)2+	3.254e-09	3.031e-09	-8.488	-8.518	-0.031	(0)
AlOH+2	1.953e-11	1.470e-11	-10.709	-10.833	-0.123	-27.24
Al+3	7.592e-14	4.184e-14	-13.120	-13.378	-0.259	-41.29
AlSO4+	2.836e-14	2.638e-14	-13.547	-13.579	-0.031	(0)
Al(SO4)2-	1.968e-16	1.830e-16	-15.706	-15.737	-0.031	(0)
AlHSO4+2	3.893e-23	2.909e-23	-22.410	-22.536	-0.127	(0)
Ba	5.098e-07					
Ba+2	4.639e-07	3.469e-07	-6.334	-6.460	-0.126	-13.38
BaSO4	4.021e-08	4.025e-08	-7.396	-7.395	0.000	(0)
BaHCO3+	4.968e-09	4.618e-09	-8.304	-8.336	-0.032	(0)
BaCO3	7.578e-10	7.587e-10	-9.120	-9.120	0.000	-10.82

BaOH+	9.360e-13	8.714e-13	-12.029	-12.060	-0.031	(0)
C(4)	2.218e-03					
HCO3-	2.115e-03	1.970e-03	-2.675	-2.706	-0.031	23.69
CO2	7.110e-05	7.118e-05	-4.148	-4.148	0.000	32.23
CaHCO3+	1.541e-05	1.436e-05	-4.812	-4.843	-0.030	9.19
CO3-2	7.027e-06	5.290e-06	-5.153	-5.277	-0.123	-6.47
CaCO3	5.292e-06	5.298e-06	-5.276	-5.276	0.000	-14.64
MgHCO3+	2.860e-06	2.659e-06	-5.544	-5.575	-0.032	5.12
NaHCO3	1.355e-06	1.356e-06	-5.868	-5.868	0.000	1.80
MgCO3	5.085e-07	5.091e-07	-6.294	-6.293	0.000	-17.08
PbCO3	1.174e-07	1.175e-07	-6.931	-6.930	0.000	(0)
CuCO3	9.142e-08	9.152e-08	-7.039	-7.038	0.000	(0)
NaCO3-	6.795e-08	6.318e-08	-7.168	-7.199	-0.032	-2.32
BaHCO3+	4.968e-09	4.618e-09	-8.304	-8.336	-0.032	(0)
CuHCO3+	3.421e-09	3.180e-09	-8.466	-8.498	-0.032	(0)
PbHCO3+	2.150e-09	1.999e-09	-8.667	-8.699	-0.032	(0)
Pb(CO3)2-2	2.089e-09	1.561e-09	-8.680	-8.807	-0.127	(0)
Cu(CO3)2-2	8.157e-10	6.095e-10	-9.088	-9.215	-0.127	(0)
BaCO3	7.578e-10	7.587e-10	-9.120	-9.120	0.000	-10.82
Ca	9.898e-04					
Ca+2	9.423e-04	7.090e-04	-3.026	-3.149	-0.124	-18.22
CaSO4	2.674e-05	2.677e-05	-4.573	-4.572	0.000	7.01
CaHCO3+	1.541e-05	1.436e-05	-4.812	-4.843	-0.030	9.19
CaCO3	5.292e-06	5.298e-06	-5.276	-5.276	0.000	-14.64
CaOH+	9.381e-09	8.722e-09	-8.028	-8.059	-0.032	(0)
CaHSO4+	2.210e-12	2.055e-12	-11.656	-11.687	-0.032	(0)
Cl	4.063e-04					
Cl-	4.063e-04	3.775e-04	-3.391	-3.423	-0.032	17.65
PbCl+	1.552e-11	1.443e-11	-10.809	-10.841	-0.032	7.49
CuCl2-	7.565e-12	7.032e-12	-11.121	-11.153	-0.032	(0)
CuCl+	2.002e-12	1.861e-12	-11.698	-11.730	-0.032	4.07
PbCl2	1.070e-14	1.071e-14	-13.971	-13.970	0.000	33.91
CuCl3-2	5.359e-15	4.025e-15	-14.271	-14.395	-0.124	(0)
CuCl2	3.328e-16	3.332e-16	-15.478	-15.477	0.000	15.77
PbCl3-	3.217e-18	2.991e-18	-17.493	-17.524	-0.032	64.36
PbCl4-2	6.619e-22	4.946e-22	-21.179	-21.306	-0.127	99.29
CuCl3-	3.914e-22	3.638e-22	-21.407	-21.439	-0.032	(0)
CuCl4-2	7.018e-28	5.271e-28	-27.154	-27.278	-0.124	(0)
Cu(1)	1.713e-10					
Cu+	1.637e-10	1.518e-10	-9.786	-9.819	-0.033	(0)
CuCl2-	7.565e-12	7.032e-12	-11.121	-11.153	-0.032	(0)
CuCl3-2	5.359e-15	4.025e-15	-14.271	-14.395	-0.124	(0)
Cu(2)	4.721e-07					
Cu(OH)2	3.694e-07	3.698e-07	-6.432	-6.432	0.000	(0)
CuCO3	9.142e-08	9.152e-08	-7.039	-7.038	0.000	(0)
Cu+2	4.265e-09	3.222e-09	-8.370	-8.492	-0.122	-26.44
CuHCO3+	3.421e-09	3.180e-09	-8.466	-8.498	-0.032	(0)
CuOH+	2.569e-09	2.388e-09	-8.590	-8.622	-0.032	(0)
Cu(CO3)2-2	8.157e-10	6.095e-10	-9.088	-9.215	-0.127	(0)
CuSO4	1.405e-10	1.406e-10	-9.852	-9.852	0.000	11.45
CuCl+	2.002e-12	1.861e-12	-11.698	-11.730	-0.032	4.07
Cu(OH)3-	1.777e-12	1.652e-12	-11.750	-11.782	-0.032	(0)
Cu2(OH)2+2	1.063e-12	7.943e-13	-11.973	-12.100	-0.127	(0)
CuCl2	3.328e-16	3.332e-16	-15.478	-15.477	0.000	15.77
Cu(OH)4-2	3.269e-17	2.443e-17	-16.486	-16.612	-0.127	(0)
CuCl3-	3.914e-22	3.638e-22	-21.407	-21.439	-0.032	(0)
CuCl4-2	7.018e-28	5.271e-28	-27.154	-27.278	-0.124	(0)
H(0)	2.887e-27					
H2	1.443e-27	1.445e-27	-26.841	-26.840	0.000	28.62
K	9.644e-05					
K+	9.631e-05	8.947e-05	-4.016	-4.048	-0.032	8.61
KSO4-	1.278e-07	1.190e-07	-6.894	-6.924	-0.031	33.76
Mg	1.666e-04					
Mg+2	1.584e-04	1.196e-04	-3.800	-3.922	-0.122	-21.29
MgSO4	4.817e-06	4.823e-06	-5.317	-5.317	0.000	5.34
MgHCO3+	2.860e-06	2.659e-06	-5.544	-5.575	-0.032	5.12
MgCO3	5.085e-07	5.091e-07	-6.294	-6.293	0.000	-17.08
MgOH+	1.218e-08	1.136e-08	-7.914	-7.944	-0.030	(0)

Na	1.236e-03					
Na+	1.233e-03	1.147e-03	-2.909	-2.940	-0.031	-2.12
NaHCO3	1.355e-06	1.356e-06	-5.868	-5.868	0.000	1.80
NaSO4-	1.328e-06	1.237e-06	-5.877	-5.908	-0.031	14.25
NaCO3-	6.795e-08	6.318e-08	-7.168	-7.199	-0.032	-2.32
NaOH	3.510e-20	3.514e-20	-19.455	-19.454	0.000	(0)
O(0)	4.457e-04					
O2	2.229e-04	2.231e-04	-3.652	-3.651	0.000	29.39
Pb	1.255e-07					
PbCO3	1.174e-07	1.175e-07	-6.931	-6.930	0.000	(0)
PbHCO3+	2.150e-09	1.999e-09	-8.667	-8.699	-0.032	(0)
Pb(CO3)2-2	2.089e-09	1.561e-09	-8.680	-8.807	-0.127	(0)
PbOH+	1.987e-09	1.847e-09	-8.702	-8.734	-0.032	(0)
Pb+2	1.710e-09	1.278e-09	-8.767	-8.893	-0.127	-15.34
PbSO4	1.662e-10	1.664e-10	-9.779	-9.779	0.000	(0)
Pb(OH)2	5.320e-11	5.326e-11	-10.274	-10.274	0.000	(0)
PbCl+	1.552e-11	1.443e-11	-10.809	-10.841	-0.032	7.49
Pb(SO4)2-2	2.705e-13	2.021e-13	-12.568	-12.694	-0.127	(0)
Pb(OH)3-	4.876e-14	4.533e-14	-13.312	-13.344	-0.032	(0)
PbCl2	1.070e-14	1.071e-14	-13.971	-13.970	0.000	33.91
Pb2OH+3	1.018e-16	5.284e-17	-15.992	-16.277	-0.285	(0)
Pb(OH)4-2	1.030e-17	7.697e-18	-16.987	-17.114	-0.127	(0)
PbCl3-	3.217e-18	2.991e-18	-17.493	-17.524	-0.032	64.36
Pb3(OH)4+2	1.972e-20	1.473e-20	-19.705	-19.832	-0.127	(0)
PbCl4-2	6.619e-22	4.946e-22	-21.179	-21.306	-0.127	99.29
S(6)	3.414e-04					
SO4-2	3.084e-04	2.315e-04	-3.511	-3.635	-0.125	12.78
CaSO4	2.674e-05	2.677e-05	-4.573	-4.572	0.000	7.01
MgSO4	4.817e-06	4.823e-06	-5.317	-5.317	0.000	5.34
NaSO4-	1.328e-06	1.237e-06	-5.877	-5.908	-0.031	14.25
KSO4-	1.278e-07	1.190e-07	-6.894	-6.924	-0.031	33.76
BaSO4	4.021e-08	4.025e-08	-7.396	-7.395	0.000	(0)
HSO4-	2.593e-10	2.411e-10	-9.586	-9.618	-0.032	39.37
PbSO4	1.662e-10	1.664e-10	-9.779	-9.779	0.000	(0)
CuSO4	1.405e-10	1.406e-10	-9.852	-9.852	0.000	11.45
CaHSO4+	2.210e-12	2.055e-12	-11.656	-11.687	-0.032	(0)
Pb(SO4)2-2	2.705e-13	2.021e-13	-12.568	-12.694	-0.127	(0)
AlSO4+	2.836e-14	2.638e-14	-13.547	-13.579	-0.031	(0)
Al(SO4)2-	1.968e-16	1.830e-16	-15.706	-15.737	-0.031	(0)
AlHSO4+2	3.893e-23	2.909e-23	-22.410	-22.536	-0.127	(0)
Si	2.033e-04					
H4SiO4	2.017e-04	2.019e-04	-3.695	-3.695	0.000	53.18
H3SiO4-	1.567e-06	1.457e-06	-5.805	-5.837	-0.032	27.62
H2SiO4-2	4.507e-12	3.393e-12	-11.346	-11.469	-0.123	(0)

----------Saturation indices----------

Phase	SI**	log IAP	log K(287 K, 1 atm)	
Al(OH)3(a)	-1.32	10.23	11.55	Al(OH)3
Albite	-1.06	-19.79	-18.74	NaAlSi3O8
Alunite	-4.26	-4.23	0.02	KAl3(SO4)2(OH)6
Anglesite	-4.68	-12.53	-7.85	PbSO4
Anhydrite	-2.62	-6.78	-4.16	CaSO4
Anorthite	-2.03	-22.07	-20.04	CaAl2Si2O8
Aragonite	-0.15	-8.43	-8.27	CaCO3
Barite	0.07	-10.10	-10.17	BaSO4
Ca-Montmorillonite	3.42	-43.26	-46.68	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	-0.00	-8.43	-8.43	CaCO3
Cerrusite	-0.90	-14.17	-13.27	PbCO3
Chalcedony	-0.01	-3.69	-3.69	SiO2
Chlorite(14A)	-4.21	68.47	72.67	Mg5Al2Si3O10(OH)8
Chrysotile	-5.56	28.06	33.63	Mg3Si2O5(OH)4
CO2(g)	-2.83	-4.15	-1.32	CO2
Dolomite	-0.80	-17.62	-16.82	CaMg(CO3)2
Gibbsite	1.48	10.23	8.76	Al(OH)3
Gypsum	-2.20	-6.78	-4.59	CaSO4:2H2O
H2(g)	-23.77	-26.84	-3.07	H2

```
  H2O(g)           -1.80     -0.00    1.80  H2O
  Halite           -7.92     -6.36    1.56  NaCl
  Illite            2.77    -39.05  -41.82  K0.6Mg0.25Al2.3Si3.5O10(OH)2
  K-feldspar        0.55    -20.90  -21.45  KAlSi3O8
  K-mica            9.05     23.43   14.39  KAl3Si3O10(OH)2
  Kaolinite         4.64     13.07    8.44  Al2Si2O5(OH)4
  O2(g)            -0.85     -3.65   -2.80  O2
  Pb(OH)2          -1.70      6.85    8.55  Pb(OH)2
  Quartz            0.46     -3.69   -4.15  SiO2
  Sepiolite        -3.51     12.55   16.06  Mg2Si3O7.5OH:3H2O
  Sepiolite(d)     -6.11     12.55   18.66  Mg2Si3O7.5OH:3H2O
  SiO2(a)          -0.89     -3.69   -2.81  SiO2
  Sylvite          -8.31     -7.47    0.84  KCl
  Talc             -2.04     20.67   22.71  Mg3Si4O10(OH)2
  Witherite        -3.13    -11.74   -8.60  BaCO3

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
  For ideal gases, phi = 1.

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End of simulation.
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Reading input data for simulation 2.
-----------------------------------

      TITLE Mixing Scenario Part II
      SOLUTION 2  DI Extraction
            units   ppm
            temp    25.0
            pH    8.6
            O(0)            5.0
            Ca              3.97
            Mg              0.46
            Na              1.15
            K               0.55
            Ba              0.07
            Be              0.08
            Cd              0.007
            Cu              0.05
            Pb              0.04
            Mn              0.01
            Se              0.02
            Ni              0.01
            Fe              0.042
            Al              0.77
            As              0.04
            Cl              1.56
            Alkalinity      12.83 as HCO3
            S(6)        4.81
            Si    2.79
      END
-----
TITLE
-----

 Mixing Scenario Part II

WARNING: Could not find element in database, As.
      Concentration is set to zero.
WARNING: Could not find element in database, Be.
      Concentration is set to zero.
WARNING: Could not find element in database, Ni.
      Concentration is set to zero.
WARNING: Could not find element in database, Se.
      Concentration is set to zero.
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```

Beginning of initial solution calculations.

Initial solution 2. DI Extraction

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

Elements	Molality	Moles
Al	2.854e-05	2.854e-05
Alkalinity	2.103e-04	2.103e-04
Ba	5.097e-07	5.097e-07
Ca	9.906e-05	9.906e-05
Cd	6.228e-08	6.228e-08
Cl	4.400e-05	4.400e-05
Cu	7.869e-07	7.869e-07
Fe	7.521e-07	7.521e-07
K	1.407e-05	1.407e-05
Mg	1.892e-05	1.892e-05
Mn	1.820e-07	1.820e-07
Na	5.002e-05	5.002e-05
O(0)	3.125e-04	3.125e-04
Pb	1.931e-07	1.931e-07
S(6)	5.007e-05	5.007e-05
Si	4.644e-05	4.644e-05

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

pH	= 8.600
pe	= 4.000
Specific Conductance (µS/cm, 25°C)	= 32
Density (g/cm³)	= 0.99706
Volume (L)	= 1.00297
Activity of water	= 1.000
Ionic strength	= 4.496e-04
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 8.518e-05
Total CO2 (mol/kg)	= 8.518e-05
Temperature (°C)	= 25.00
Electrical balance (eq)	= 3.546e-05
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 6.30
Iterations	= 9
Total H	= 1.110128e+02
Total O	= 5.550729e+01

-----Redox couples-----

Redox couple	pe	Eh (volts)
O(-2)/O(0)	11.9685	0.7080

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	4.129e-06	4.029e-06	-5.384	-5.395	-0.011	-4.12
H+	2.571e-09	2.512e-09	-8.590	-8.600	-0.010	0.00
H2O	5.551e+01	1.000e+00	1.744	-0.000	0.000	18.07
Al	2.854e-05					
Al(OH)4-	2.850e-05	2.782e-05	-4.545	-4.556	-0.010	(0)
Al(OH)3	3.708e-08	3.708e-08	-7.431	-7.431	0.000	(0)
Al(OH)2+	6.475e-10	6.321e-10	-9.189	-9.199	-0.010	(0)
AlOH+2	2.230e-13	2.026e-13	-12.652	-12.693	-0.042	-27.80
Al+3	6.326e-17	5.123e-17	-16.199	-16.290	-0.092	-42.36
AlSO4+	7.410e-18	7.233e-18	-17.130	-17.141	-0.010	(0)
Al(SO4)2-	1.046e-20	1.021e-20	-19.980	-19.991	-0.010	(0)
AlHSO4+2	1.775e-27	1.611e-27	-26.751	-26.793	-0.042	(0)

Ba	5.097e-07					
Ba+2	4.989e-07	4.528e-07	-6.302	-6.344	-0.042	-12.78
BaSO4	1.013e-08	1.013e-08	-7.994	-7.994	0.000	(0)
BaHCO3+	3.584e-10	3.498e-10	-9.446	-9.456	-0.011	(0)
BaCO3	3.520e-10	3.520e-10	-9.454	-9.453	0.000	-10.70
BaOH+	6.257e-12	6.109e-12	-11.204	-11.214	-0.010	(0)
C(4)	8.518e-05					
HCO3-	8.254e-05	8.059e-05	-4.083	-4.094	-0.010	24.67
CO3-2	1.656e-06	1.505e-06	-5.781	-5.823	-0.042	-5.31
CO2	4.551e-07	4.551e-07	-6.342	-6.342	0.000	29.09
CaCO3	2.250e-07	2.251e-07	-6.648	-6.648	0.000	-14.60
PbCO3	1.379e-07	1.379e-07	-6.860	-6.860	0.000	(0)
CaHCO3+	9.377e-08	9.155e-08	-7.028	-7.038	-0.010	9.66
MgCO3	2.437e-08	2.437e-08	-7.613	-7.613	0.000	-17.09
MnCO3	1.746e-08	1.746e-08	-7.758	-7.758	0.000	(0)
MgHCO3+	1.640e-08	1.600e-08	-7.785	-7.796	-0.011	5.47
NaHCO3	2.212e-09	2.212e-09	-8.655	-8.655	0.000	1.80
CuCO3	1.912e-09	1.912e-09	-8.718	-8.718	0.000	(0)
NaCO3-	1.401e-09	1.368e-09	-8.853	-8.864	-0.011	-1.04
MnHCO3+	1.075e-09	1.049e-09	-8.969	-8.979	-0.010	(0)
Pb(CO3)2-2	5.742e-10	5.212e-10	-9.241	-9.283	-0.042	(0)
BaHCO3+	3.584e-10	3.498e-10	-9.446	-9.456	-0.011	(0)
BaCO3	3.520e-10	3.520e-10	-9.454	-9.453	0.000	-10.70
PbHCO3+	3.459e-10	3.376e-10	-9.461	-9.472	-0.011	(0)
CdHCO3+	1.404e-10	1.371e-10	-9.853	-9.863	-0.011	(0)
CdCO3	6.427e-11	6.428e-11	-10.192	-10.192	0.000	(0)
CuHCO3+	9.794e-12	9.560e-12	-11.009	-11.020	-0.011	(0)
Cu(CO3)2-2	3.991e-12	3.623e-12	-11.399	-11.441	-0.042	(0)
FeCO3	1.175e-12	1.175e-12	-11.930	-11.930	0.000	(0)
Cd(CO3)2-2	3.369e-13	3.058e-13	-12.472	-12.515	-0.042	(0)
FeHCO3+	2.688e-13	2.624e-13	-12.571	-12.581	-0.011	(0)
Ca	9.906e-05					
Ca+2	9.802e-05	8.904e-05	-4.009	-4.050	-0.042	-18.18
CaSO4	7.069e-07	7.070e-07	-6.151	-6.151	0.000	7.50
CaCO3	2.250e-07	2.251e-07	-6.648	-6.648	0.000	-14.60
CaHCO3+	9.377e-08	9.155e-08	-7.028	-7.038	-0.010	9.66
CaOH+	6.027e-09	5.883e-09	-8.220	-8.230	-0.011	(0)
CaHSO4+	1.196e-14	1.167e-14	-13.922	-13.933	-0.011	(0)
Cd	6.228e-08					
Cd+2	5.926e-08	5.378e-08	-7.227	-7.269	-0.042	-18.79
CdOH+	1.825e-09	1.781e-09	-8.739	-8.749	-0.011	(0)
CdSO4	6.925e-10	6.925e-10	-9.160	-9.160	0.000	78.05
CdCl+	2.260e-10	2.206e-10	-9.646	-9.656	-0.011	5.82
CdHCO3+	1.404e-10	1.371e-10	-9.853	-9.863	-0.011	(0)
CdCO3	6.427e-11	6.428e-11	-10.192	-10.192	0.000	(0)
Cd(OH)2	3.807e-11	3.808e-11	-10.419	-10.419	0.000	(0)
CdOHCl	3.627e-11	3.627e-11	-10.440	-10.440	0.000	(0)
Cd(SO4)2-2	3.735e-13	3.390e-13	-12.428	-12.470	-0.042	-105.68
Cd(CO3)2-2	3.369e-13	3.058e-13	-12.472	-12.515	-0.042	(0)
CdCl2	3.949e-14	3.949e-14	-13.404	-13.403	0.000	23.14
Cd(OH)3-	1.742e-15	1.701e-15	-14.759	-14.769	-0.011	(0)
Cd2OH+3	5.834e-16	4.691e-16	-15.234	-15.329	-0.095	(0)
CdCl3-	1.096e-18	1.070e-18	-17.960	-17.971	-0.011	69.31
Cd(OH)4-2	6.648e-21	6.034e-21	-20.177	-20.219	-0.042	(0)
Cl	4.400e-05					
Cl-	4.400e-05	4.295e-05	-4.357	-4.367	-0.011	18.06
CdCl+	2.260e-10	2.206e-10	-9.646	-9.656	-0.011	5.82
CdOHCl	3.627e-11	3.627e-11	-10.440	-10.440	0.000	(0)
MnCl+	2.619e-11	2.556e-11	-10.582	-10.592	-0.010	-3.10
PbCl+	9.239e-12	9.017e-12	-11.034	-11.045	-0.011	7.94
CdCl2	3.949e-14	3.949e-14	-13.404	-13.403	0.000	23.14
CuCl+	2.803e-14	2.736e-14	-13.552	-13.563	-0.011	0.62
CuCl2-	7.423e-15	7.246e-15	-14.129	-14.140	-0.011	(0)
FeCl+	1.978e-15	1.930e-15	-14.704	-14.714	-0.011	(0)
PbCl2	6.137e-16	6.138e-16	-15.212	-15.212	0.000	34.97
MnCl2	4.792e-16	4.793e-16	-15.319	-15.319	0.000	85.89
CdCl3-	1.096e-18	1.070e-18	-17.960	-17.971	-0.011	69.31
CuCl2	6.310e-19	6.311e-19	-18.200	-18.200	0.000	31.02

CuCl3-2	5.430e-19	4.932e-19	-18.265	-18.307	-0.042	(0)
PbCl3-	2.145e-20	2.094e-20	-19.669	-19.679	-0.011	65.94
MnCl3-	5.807e-21	5.669e-21	-20.236	-20.246	-0.010	43.34
FeCl+2	4.441e-23	4.033e-23	-22.353	-22.394	-0.042	(0)
PbCl4-2	4.742e-25	4.304e-25	-24.324	-24.366	-0.042	101.31
CuCl3-	9.852e-26	9.616e-26	-25.006	-25.017	-0.011	(0)
FeCl2+	7.925e-27	7.737e-27	-26.101	-26.111	-0.010	(0)
FeCl3	3.323e-32	3.323e-32	-31.479	-31.478	0.000	(0)
CuCl4-2	2.279e-32	2.070e-32	-31.642	-31.684	-0.042	(0)
Cu(1)	1.274e-11					
Cu+	1.273e-11	1.242e-11	-10.895	-10.906	-0.011	(0)
CuCl2-	7.423e-15	7.246e-15	-14.129	-14.140	-0.011	(0)
CuCl3-2	5.430e-19	4.932e-19	-18.265	-18.307	-0.042	(0)
Cu(2)	7.868e-07					
Cu(OH)2	7.837e-07	7.838e-07	-6.106	-6.106	0.000	(0)
CuCO3	1.912e-09	1.912e-09	-8.718	-8.718	0.000	(0)
CuOH+	9.654e-10	9.423e-10	-9.015	-9.026	-0.011	(0)
Cu+2	2.604e-10	2.367e-10	-9.584	-9.626	-0.042	-26.64
Cu(OH)3-	1.926e-11	1.880e-11	-10.715	-10.726	-0.011	(0)
CuHCO3+	9.794e-12	9.560e-12	-11.009	-11.020	-0.011	(0)
Cu(CO3)2-2	3.991e-12	3.623e-12	-11.399	-11.441	-0.042	(0)
CuSO4	2.157e-12	2.158e-12	-11.666	-11.666	0.000	13.09
Cu2(OH)2+2	4.281e-13	3.885e-13	-12.368	-12.411	-0.042	(0)
CuCl+	2.803e-14	2.736e-14	-13.552	-13.563	-0.011	0.62
Cu(OH)4-2	1.645e-15	1.493e-15	-14.784	-14.826	-0.042	(0)
CuCl2	6.310e-19	6.311e-19	-18.200	-18.200	0.000	31.02
CuCl3-	9.852e-26	9.616e-26	-25.006	-25.017	-0.011	(0)
CuCl4-2	2.279e-32	2.070e-32	-31.642	-31.684	-0.042	(0)
Fe(2)	4.174e-11					
Fe+2	3.583e-11	3.256e-11	-10.446	-10.487	-0.042	-22.17
FeOH+	4.199e-12	4.099e-12	-11.377	-11.387	-0.010	(0)
FeCO3	1.175e-12	1.175e-12	-11.930	-11.930	0.000	(0)
FeHCO3+	2.688e-13	2.624e-13	-12.571	-12.581	-0.011	(0)
FeSO4	2.585e-13	2.585e-13	-12.588	-12.588	0.000	18.97
Fe(OH)2	1.389e-14	1.389e-14	-13.857	-13.857	0.000	(0)
FeCl+	1.978e-15	1.930e-15	-14.704	-14.714	-0.011	(0)
Fe(OH)3-	2.104e-16	2.054e-16	-15.677	-15.687	-0.010	(0)
FeHSO4+	4.373e-21	4.268e-21	-20.359	-20.370	-0.011	(0)
Fe(3)	7.520e-07					
Fe(OH)3	5.403e-07	5.403e-07	-6.267	-6.267	0.000	(0)
Fe(OH)4-	2.010e-07	1.962e-07	-6.697	-6.707	-0.010	(0)
Fe(OH)2+	1.079e-08	1.054e-08	-7.967	-7.977	-0.010	(0)
FeOH+2	8.800e-14	7.993e-14	-13.056	-13.097	-0.042	(0)
Fe+3	3.840e-20	3.109e-20	-19.416	-19.507	-0.092	(0)
FeSO4+	1.559e-20	1.522e-20	-19.807	-19.818	-0.010	(0)
FeCl+2	4.441e-23	4.033e-23	-22.353	-22.394	-0.042	(0)
Fe(SO4)2-	1.523e-23	1.487e-23	-22.817	-22.828	-0.011	(0)
Fe2(OH)2+4	2.533e-25	1.719e-25	-24.596	-24.765	-0.168	(0)
FeCl2+	7.925e-27	7.737e-27	-26.101	-26.111	-0.010	(0)
FeHSO4+2	1.128e-28	1.024e-28	-27.948	-27.990	-0.042	(0)
Fe3(OH)4+5	6.936e-31	3.785e-31	-30.159	-30.422	-0.263	(0)
FeCl3	3.323e-32	3.323e-32	-31.479	-31.478	0.000	(0)
H(0)	8.933e-29					
H2	4.466e-29	4.467e-29	-28.350	-28.350	0.000	28.61
K	1.407e-05					
K+	1.406e-05	1.372e-05	-4.852	-4.863	-0.011	9.00
KSO4-	4.410e-09	4.305e-09	-8.356	-8.366	-0.010	34.09
Mg	1.892e-05					
Mg+2	1.868e-05	1.697e-05	-4.729	-4.770	-0.042	-21.86
MgSO4	1.776e-07	1.776e-07	-6.750	-6.750	0.000	5.84
MgOH+	2.512e-08	2.453e-08	-7.600	-7.610	-0.010	(0)
MgCO3	2.437e-08	2.437e-08	-7.613	-7.613	0.000	-17.09
MgHCO3+	1.640e-08	1.600e-08	-7.785	-7.796	-0.011	5.47
Mn(2)	1.820e-07					
Mn+2	1.608e-07	1.461e-07	-6.794	-6.835	-0.042	-21.34
MnCO3	1.746e-08	1.746e-08	-7.758	-7.758	0.000	(0)
MnOH+	1.532e-09	1.495e-09	-8.815	-8.825	-0.010	(0)
MnSO4	1.160e-09	1.160e-09	-8.936	-8.936	0.000	22.54

MnHCO3+	1.075e-09	1.049e-09	-8.969	-8.979	-0.010	(0)
MnCl+	2.619e-11	2.556e-11	-10.582	-10.592	-0.010	-3.10
MnCl2	4.792e-16	4.793e-16	-15.319	-15.319	0.000	85.89
Mn(OH)3-	1.497e-16	1.461e-16	-15.825	-15.835	-0.010	(0)
MnCl3-	5.807e-21	5.669e-21	-20.236	-20.246	-0.010	43.34
Mn(3)	5.576e-29					
Mn+3	5.576e-29	4.515e-29	-28.254	-28.345	-0.092	(0)
Na	5.002e-05					
Na+	5.001e-05	4.882e-05	-4.301	-4.311	-0.010	-1.49
NaSO4-	1.119e-08	1.092e-08	-7.951	-7.962	-0.010	13.65
NaHCO3	2.212e-09	2.212e-09	-8.655	-8.655	0.000	1.80
NaCO3-	1.401e-09	1.368e-09	-8.853	-8.864	-0.011	-1.04
NaOH	1.967e-20	1.967e-20	-19.706	-19.706	0.000	(0)
O(0)	3.125e-04					
O2	1.563e-04	1.563e-04	-3.806	-3.806	0.000	30.40
Pb	1.931e-07					
PbCO3	1.379e-07	1.379e-07	-6.860	-6.860	0.000	(0)
PbOH+	4.194e-08	4.094e-08	-7.377	-7.388	-0.011	(0)
Pb(OH)2	6.340e-09	6.341e-09	-8.198	-8.198	0.000	(0)
Pb+2	5.811e-09	5.274e-09	-8.236	-8.278	-0.042	-15.58
Pb(CO3)2-2	5.742e-10	5.212e-10	-9.241	-9.283	-0.042	(0)
PbHCO3+	3.459e-10	3.376e-10	-9.461	-9.472	-0.011	(0)
PbSO4	1.324e-10	1.324e-10	-9.878	-9.878	0.000	(0)
Pb(OH)3-	2.969e-11	2.898e-11	-10.527	-10.538	-0.011	(0)
PbCl+	9.239e-12	9.017e-12	-11.034	-11.045	-0.011	7.94
Pb(SO4)2-2	3.418e-14	3.103e-14	-13.466	-13.508	-0.042	(0)
Pb(OH)4-2	2.912e-14	2.643e-14	-13.536	-13.578	-0.042	(0)
Pb2OH+3	6.011e-15	4.834e-15	-14.221	-14.316	-0.095	(0)
Pb3(OH)4+2	5.352e-15	4.857e-15	-14.272	-14.314	-0.042	(0)
PbCl2	6.137e-16	6.138e-16	-15.212	-15.212	0.000	34.97
PbCl3-	2.145e-20	2.094e-20	-19.669	-19.679	-0.011	65.94
PbCl4-2	4.742e-25	4.304e-25	-24.324	-24.366	-0.042	101.31
S(6)	5.007e-05					
SO4-2	4.916e-05	4.465e-05	-4.308	-4.350	-0.042	14.47
CaSO4	7.069e-07	7.070e-07	-6.151	-6.151	0.000	7.50
MgSO4	1.776e-07	1.776e-07	-6.750	-6.750	0.000	5.84
NaSO4-	1.119e-08	1.092e-08	-7.951	-7.962	-0.010	13.65
BaSO4	1.013e-08	1.013e-08	-7.994	-7.994	0.000	(0)
KSO4-	4.410e-09	4.305e-09	-8.356	-8.366	-0.010	34.09
MnSO4	1.160e-09	1.160e-09	-8.936	-8.936	0.000	22.54
CdSO4	6.925e-10	6.925e-10	-9.160	-9.160	0.000	78.05
PbSO4	1.324e-10	1.324e-10	-9.878	-9.878	0.000	(0)
HSO4-	1.117e-11	1.090e-11	-10.952	-10.962	-0.011	40.27
CuSO4	2.157e-12	2.158e-12	-11.666	-11.666	0.000	13.09
Cd(SO4)2-2	3.735e-13	3.390e-13	-12.428	-12.470	-0.042	-105.68
FeSO4	2.585e-13	2.585e-13	-12.588	-12.588	0.000	18.97
Pb(SO4)2-2	3.418e-14	3.103e-14	-13.466	-13.508	-0.042	(0)
CaHSO4+	1.196e-14	1.167e-14	-13.922	-13.933	-0.011	(0)
AlSO4+	7.410e-18	7.233e-18	-17.130	-17.141	-0.010	(0)
FeSO4+	1.559e-20	1.522e-20	-19.807	-19.818	-0.010	(0)
Al(SO4)2-	1.046e-20	1.021e-20	-19.980	-19.991	-0.010	(0)
FeHSO4+	4.373e-21	4.268e-21	-20.359	-20.370	-0.011	(0)
Fe(SO4)2-	1.523e-23	1.487e-23	-22.817	-22.828	-0.011	(0)
AlHSO4+2	1.775e-27	1.611e-27	-26.751	-26.793	-0.042	(0)
FeHSO4+2	1.128e-28	1.024e-28	-27.948	-27.990	-0.042	(0)
Si	4.644e-05					
H4SiO4	4.380e-05	4.381e-05	-4.359	-4.358	0.000	52.08
H3SiO4-	2.635e-06	2.571e-06	-5.579	-5.590	-0.011	27.96
H2SiO4-2	7.665e-11	6.964e-11	-10.115	-10.157	-0.042	(0)

-------------------------------Saturation indices--------------------------------

Phase	SI**	log IAP	log K(298 K, 1 atm)	
Al(OH)3(a)	-1.29	9.51	10.80	Al(OH)3
Albite	-3.94	-21.94	-18.00	NaAlSi3O8
Alunite	-9.43	-10.83	-1.40	KAl3(SO4)2(OH)6
Anglesite	-4.84	-12.63	-7.79	PbSO4

```
  Anhydrite          -4.12     -8.40   -4.28  CaSO4
  Anorthite          -2.16    -21.88  -19.71  CaAl2Si2O8
  Aragonite          -1.54     -9.87   -8.34  CaCO3
  Barite             -0.72    -10.69   -9.97  BaSO4
  Ca-Montmorillonite  0.55    -44.48  -45.03  Ca0.165Al2.33Si3.67O10(OH)2
  Calcite            -1.39     -9.87   -8.48  CaCO3
  Cd(OH)2            -3.72      9.93   13.65  Cd(OH)2
  CdSiO3             -3.49      5.57    9.06  CdSiO3
  CdSO4             -11.52    -11.62   -0.10  CdSO4
  Cerrusite          -0.97    -14.10  -13.13  PbCO3
  Chalcedony         -0.81     -4.36   -3.55  SiO2
  Chlorite(14A)      -0.29     68.09   68.38  Mg5Al2Si3O10(OH)8
  Chrysotile         -3.63     28.57   32.20  Mg3Si2O5(OH)4
  CO2(g)             -4.88     -6.34   -1.46  CO2
  Dolomite           -3.38    -20.47  -17.09  CaMg(CO3)2
  Fe(OH)3(a)          1.40      6.29    4.89  Fe(OH)3
  Gibbsite            1.40      9.51    8.11  Al(OH)3
  Goethite            7.29      6.29   -1.00  FeOOH
  Gypsum             -3.82     -8.40   -4.58  CaSO4:2H2O
  H2(g)             -25.25    -28.35   -3.10  H2
  H2O(g)             -1.50     -0.00    1.50  H2O
  Halite            -10.25     -8.68    1.57  NaCl
  Hausmannite        -4.74     56.29   61.03  Mn3O4
  Hematite           16.59     12.59   -4.01  Fe2O3
  Illite              0.10    -40.16  -40.27  K0.6Mg0.25Al2.3Si3.5O10(OH)2
  Jarosite-K        -11.27    -20.48   -9.21  KFe3(SO4)2(OH)6
  K-feldspar         -1.92    -22.49  -20.57  KAlSi3O8
  K-mica              6.49     19.19   12.70  KAl3Si3O10(OH)2
  Kaolinite           2.87     10.30    7.43  Al2Si2O5(OH)4
  Manganite          -2.38     22.96   25.34  MnOOH
  Melanterite       -12.63    -14.84   -2.21  FeSO4:7H2O
  O2(g)              -0.91     -3.81   -2.89  O2
  Otavite            -0.99    -13.09  -12.10  CdCO3
  Pb(OH)2             0.77      8.92    8.15  Pb(OH)2
  Pyrochroite        -4.84     10.36   15.20  Mn(OH)2
  Pyrolusite         -5.82     35.56   41.38  MnO2:H2O
  Quartz             -0.38     -4.36   -3.98  SiO2
  Rhodochrosite      -1.53    -12.66  -11.13  MnCO3
  Sepiolite          -3.98     11.78   15.76  Mg2Si3O7.5OH:3H2O
  Sepiolite(d)       -6.88     11.78   18.66  Mg2Si3O7.5OH:3H2O
  Siderite           -5.42    -16.31  -10.89  FeCO3
  SiO2(a)            -1.65     -4.36   -2.71  SiO2
  Sylvite           -10.13     -9.23    0.90  KCl
  Talc               -1.54     19.86   21.40  Mg3Si4O10(OH)2
  Witherite          -3.60    -12.17   -8.56  BaCO3

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
  For ideal gases, phi = 1.

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End of simulation.
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Reading input data for simulation 3.
------------------------------------

      TITLE Aqua Mix part III: mix 95% soln 1, 5% soln 2.
      MIX 1
              1      0.95
              2      0.05
      SAVE solution   3
      END
-----
TITLE
-----

 Aqua Mix part III: mix 95% soln 1, 5% soln 2.
```

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

Reaction step 1.

Using mix 1.

Mixture 1.

        9.500e-01 Solution 1  MW-4
        5.000e-02 Solution 2  DI Extraction

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

      Elements           Molality       Moles

      Al                3.188e-06   3.188e-06
      Ba                5.098e-07   5.098e-07
      C                 2.112e-03   2.112e-03
      Ca                9.453e-04   9.453e-04
      Cd                3.114e-09   3.114e-09
      Cl                3.882e-04   3.882e-04
      Cu                4.880e-07   4.880e-07
      Fe                3.760e-08   3.760e-08
      K                 9.232e-05   9.232e-05
      Mg                1.592e-04   1.592e-04
      Mn                9.101e-09   9.101e-09
      Na                1.176e-03   1.176e-03
      Pb                1.289e-07   1.289e-07
      S                 3.269e-04   3.269e-04
      Si                1.954e-04   1.954e-04

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

                                     pH  =   7.869      Charge balance
                                     pe  =  13.642      Adjusted to redox equilibrium
       Specific Conductance (µS/cm, 14°C)  = 254
                            Density (g/cm³)  =   0.99939
                                 Volume (L)  =   1.00088
                          Activity of water  =   1.000
                             Ionic strength  =   4.558e-03
                         Mass of water (kg)  =   1.000e+00
                 Total alkalinity (eq/kg)  =   2.072e-03
                         Total CO2 (mol/kg)  =   2.112e-03
                           Temperature (°C)  =  14.46
                  Electrical balance (eq)  =   3.753e-04
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   5.86
                                Iterations  =  18
                                   Total H  = 1.110153e+02
                                   Total O  = 5.551503e+01

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

                                                 Log       Log       Log    mole V
   Species          Molality    Activity  Molality  Activity     Gamma   cm³/mol

   OH-             3.448e-07   3.207e-07    -6.462    -6.494    -0.031     -4.63
   H+              1.441e-08   1.351e-08    -7.841    -7.869    -0.028      0.00
   H2O             5.551e+01   9.999e-01     1.744    -0.000     0.000     18.03
Al            3.188e-06
   Al(OH)4-        3.159e-06   2.943e-06    -5.500    -5.531    -0.031       (0)
   Al(OH)3         2.353e-08   2.355e-08    -7.628    -7.628     0.000       (0)
   Al(OH)2+        5.331e-09   4.972e-09    -8.273    -8.303    -0.030       (0)
   AlOH+2          3.020e-11   2.286e-11   -10.520   -10.641    -0.121    -27.27
   Al+3            1.125e-13   6.269e-14   -12.949   -13.203    -0.254    -41.34
   AlSO4+          4.127e-14   3.845e-14   -13.384   -13.415    -0.031       (0)
```

Al(SO4)2-	2.772e-16	2.583e-16	-15.557	-15.588	-0.031	(0)
AlHSO4+2	5.667e-23	4.259e-23	-22.247	-22.371	-0.124	(0)
Ba	5.098e-07					
Ba+2	4.651e-07	3.498e-07	-6.332	-6.456	-0.124	-13.33
BaSO4	3.914e-08	3.918e-08	-7.407	-7.407	0.000	(0)
BaHCO3+	4.854e-09	4.520e-09	-8.314	-8.345	-0.031	(0)
BaCO3	7.469e-10	7.477e-10	-9.127	-9.126	0.000	-10.81
BaOH+	9.413e-13	8.775e-13	-12.026	-12.057	-0.030	(0)
C(-4)	0.000e+00					
CH4	0.000e+00	0.000e+00	-150.408	-150.408	0.000	32.22
C(4)	2.112e-03					
HCO3-	2.014e-03	1.878e-03	-2.696	-2.726	-0.030	23.75
CO2	6.717e-05	6.724e-05	-4.173	-4.172	0.000	32.04
CaHCO3+	1.430e-05	1.335e-05	-4.845	-4.875	-0.030	9.22
CO3-2	6.755e-06	5.113e-06	-5.170	-5.291	-0.121	-6.38
CaCO3	4.948e-06	4.954e-06	-5.306	-5.305	0.000	-14.64
MgHCO3+	2.623e-06	2.442e-06	-5.581	-5.612	-0.031	5.14
NaHCO3	1.228e-06	1.229e-06	-5.911	-5.910	0.000	1.80
MgCO3	4.769e-07	4.774e-07	-6.322	-6.321	0.000	-17.08
PbCO3	1.205e-07	1.206e-07	-6.919	-6.919	0.000	(0)
CuCO3	9.217e-08	9.226e-08	-7.035	-7.035	0.000	(0)
NaCO3-	6.445e-08	6.000e-08	-7.191	-7.222	-0.031	-2.23
BaHCO3+	4.854e-09	4.520e-09	-8.314	-8.345	-0.031	(0)
CuHCO3+	3.397e-09	3.163e-09	-8.469	-8.500	-0.031	(0)
PbHCO3+	2.176e-09	2.026e-09	-8.662	-8.693	-0.031	(0)
Pb(CO3)2-2	2.062e-09	1.549e-09	-8.686	-8.810	-0.124	(0)
MnCO3	1.907e-09	1.909e-09	-8.720	-8.719	0.000	(0)
MnHCO3+	8.439e-10	7.867e-10	-9.074	-9.104	-0.030	(0)
Cu(CO3)2-2	7.903e-10	5.939e-10	-9.102	-9.226	-0.124	(0)
BaCO3	7.469e-10	7.477e-10	-9.127	-9.126	0.000	-10.81
CdHCO3+	1.326e-10	1.234e-10	-9.878	-9.909	-0.031	(0)
CdCO3	8.431e-12	8.440e-12	-11.074	-11.074	0.000	(0)
Cd(CO3)2-2	1.816e-13	1.365e-13	-12.741	-12.865	-0.124	(0)
FeHCO3+	1.117e-19	1.040e-19	-18.952	-18.983	-0.031	(0)
FeCO3	6.783e-20	6.791e-20	-19.169	-19.168	0.000	(0)
Ca	9.453e-04					
Ca+2	9.011e-04	6.817e-04	-3.045	-3.166	-0.121	-18.21
CaSO4	2.493e-05	2.496e-05	-4.603	-4.603	0.000	7.04
CaHCO3+	1.430e-05	1.335e-05	-4.845	-4.875	-0.030	9.22
CaCO3	4.948e-06	4.954e-06	-5.306	-5.305	0.000	-14.64
CaOH+	8.996e-09	8.376e-09	-8.046	-8.077	-0.031	(0)
CaHSO4+	2.073e-12	1.931e-12	-11.683	-11.714	-0.031	(0)
Cd	3.114e-09					
Cd+2	2.765e-09	2.078e-09	-8.558	-8.682	-0.124	-19.27
CdHCO3+	1.326e-10	1.234e-10	-9.878	-9.909	-0.031	(0)
CdSO4	1.251e-10	1.253e-10	-9.903	-9.902	0.000	84.16
CdCl+	7.423e-11	6.911e-11	-10.129	-10.160	-0.031	2.69
CdCO3	8.431e-12	8.440e-12	-11.074	-11.074	0.000	(0)
CdOH+	6.110e-12	5.689e-12	-11.214	-11.245	-0.031	(0)
CdOHCl	1.672e-12	1.674e-12	-11.777	-11.776	0.000	(0)
Cd(SO4)2-2	4.366e-13	3.281e-13	-12.360	-12.484	-0.124	-113.88
Cd(CO3)2-2	1.816e-13	1.365e-13	-12.741	-12.865	-0.124	(0)
CdCl2	9.986e-14	9.997e-14	-13.001	-13.000	0.000	23.14
Cd(OH)2	5.082e-14	5.087e-14	-13.294	-13.294	0.000	(0)
CdCl3-	2.076e-17	1.933e-17	-16.683	-16.714	-0.031	78.20
Cd(OH)3-	4.539e-19	4.226e-19	-18.343	-18.374	-0.031	(0)
Cd2OH+3	1.262e-19	6.634e-20	-18.899	-19.178	-0.279	(0)
Cd(OH)4-2	3.710e-25	2.788e-25	-24.431	-24.555	-0.124	(0)
CdHS+	0.000e+00	0.000e+00	-146.824	-146.855	-0.031	(0)
Cd(HS)2	0.000e+00	0.000e+00	-288.839	-288.838	0.000	(0)
Cd(HS)3-	0.000e+00	0.000e+00	-434.970	-435.001	-0.031	(0)
Cd(HS)4-2	0.000e+00	0.000e+00	-581.030	-581.154	-0.124	(0)
Cl	3.882e-04					
Cl-	3.882e-04	3.612e-04	-3.411	-3.442	-0.031	17.68
CdCl+	7.423e-11	6.911e-11	-10.129	-10.160	-0.031	2.69
PbCl+	1.599e-11	1.489e-11	-10.796	-10.827	-0.031	7.52
MnCl+	7.418e-12	6.915e-12	-11.130	-11.160	-0.030	-6.27
CuCl+	2.055e-12	1.913e-12	-11.687	-11.718	-0.031	3.87

CdOHCl	1.672e-12	1.674e-12	-11.777	-11.776	0.000	(0)
CdCl2	9.986e-14	9.997e-14	-13.001	-13.000	0.000	23.14
PbCl2	1.044e-14	1.045e-14	-13.981	-13.981	0.000	33.97
MnCl2	1.089e-15	1.090e-15	-14.963	-14.962	0.000	101.08
CuCl2	3.293e-16	3.297e-16	-15.482	-15.482	0.000	16.67
CdCl3-	2.076e-17	1.933e-17	-16.683	-16.714	-0.031	78.20
PbCl3-	3.011e-18	2.804e-18	-17.521	-17.552	-0.031	64.46
MnCl3-	1.164e-19	1.085e-19	-18.934	-18.965	-0.030	43.76
FeCl+2	1.300e-20	9.817e-21	-19.886	-20.008	-0.122	(0)
CuCl2-	1.653e-21	1.539e-21	-20.782	-20.813	-0.031	(0)
PbCl4-2	5.930e-22	4.456e-22	-21.227	-21.351	-0.124	99.42
CuCl3-	3.740e-22	3.481e-22	-21.427	-21.458	-0.031	(0)
FeCl+	2.965e-22	2.760e-22	-21.528	-21.559	-0.031	(0)
FeCl2+	2.403e-23	2.240e-23	-22.619	-22.650	-0.030	(0)
CuCl3-2	1.118e-24	8.446e-25	-23.951	-24.073	-0.122	(0)
FeCl3	8.083e-28	8.091e-28	-27.092	-27.092	0.000	(0)
CuCl4-2	6.479e-28	4.893e-28	-27.189	-27.310	-0.122	(0)
Cu(1)	4.078e-20					
Cu+	3.912e-20	3.634e-20	-19.408	-19.440	-0.032	(0)
CuCl2-	1.653e-21	1.539e-21	-20.782	-20.813	-0.031	(0)
CuCl3-2	1.118e-24	8.446e-25	-23.951	-24.073	-0.122	(0)
Cu(2)	4.880e-07					
Cu(OH)2	3.844e-07	3.848e-07	-6.415	-6.415	0.000	(0)
CuCO3	9.217e-08	9.226e-08	-7.035	-7.035	0.000	(0)
Cu+2	4.425e-09	3.360e-09	-8.354	-8.474	-0.120	-26.45
CuHCO3+	3.397e-09	3.163e-09	-8.469	-8.500	-0.031	(0)
CuOH+	2.672e-09	2.488e-09	-8.573	-8.604	-0.031	(0)
Cu(CO3)2-2	7.903e-10	5.939e-10	-9.102	-9.226	-0.124	(0)
CuSO4	1.420e-10	1.422e-10	-9.848	-9.847	0.000	11.55
CuCl+	2.055e-12	1.913e-12	-11.687	-11.718	-0.031	3.87
Cu(OH)3-	1.843e-12	1.716e-12	-11.734	-11.765	-0.031	(0)
Cu2(OH)2+2	1.217e-12	9.146e-13	-11.915	-12.039	-0.124	(0)
CuCl2	3.293e-16	3.297e-16	-15.482	-15.482	0.000	16.67
Cu(OH)4-2	3.374e-17	2.535e-17	-16.472	-16.596	-0.124	(0)
CuCl3-	3.740e-22	3.481e-22	-21.427	-21.458	-0.031	(0)
CuCl4-2	6.479e-28	4.893e-28	-27.189	-27.310	-0.122	(0)
Cu(HS)3-	0.000e+00	0.000e+00	-427.571	-427.602	-0.031	(0)
Fe(2)	9.330e-19					
Fe+2	7.290e-19	5.536e-19	-18.137	-18.257	-0.120	-22.80
FeHCO3+	1.117e-19	1.040e-19	-18.952	-18.983	-0.031	(0)
FeCO3	6.783e-20	6.791e-20	-19.169	-19.168	0.000	(0)
FeSO4	1.800e-20	1.801e-20	-19.745	-19.744	0.000	31.95
FeOH+	6.143e-21	5.727e-21	-20.212	-20.242	-0.030	(0)
FeCl+	2.965e-22	2.760e-22	-21.528	-21.559	-0.031	(0)
Fe(OH)2	1.393e-24	1.394e-24	-23.856	-23.856	0.000	(0)
Fe(OH)3-	3.695e-27	3.445e-27	-26.432	-26.463	-0.030	(0)
FeHSO4+	1.684e-27	1.568e-27	-26.774	-26.805	-0.031	(0)
Fe(HS)2	0.000e+00	0.000e+00	-305.993	-305.993	0.000	(0)
Fe(HS)3-	0.000e+00	0.000e+00	-452.267	-452.298	-0.031	(0)
Fe(3)	3.760e-08					
Fe(OH)3	3.062e-08	3.066e-08	-7.514	-7.513	0.000	(0)
Fe(OH)2+	5.550e-09	5.176e-09	-8.256	-8.286	-0.030	(0)
Fe(OH)4-	1.430e-09	1.334e-09	-8.845	-8.875	-0.030	(0)
FeOH+2	4.232e-13	3.196e-13	-12.373	-12.495	-0.122	(0)
FeSO4+	2.626e-18	2.448e-18	-17.581	-17.611	-0.030	(0)
Fe+3	2.285e-18	1.273e-18	-17.641	-17.895	-0.254	(0)
FeCl+2	1.300e-20	9.817e-21	-19.886	-20.008	-0.122	(0)
Fe(SO4)2-	1.232e-20	1.147e-20	-19.909	-19.940	-0.031	(0)
FeCl2+	2.403e-23	2.240e-23	-22.619	-22.650	-0.030	(0)
Fe2(OH)2+4	1.354e-23	4.320e-24	-22.868	-23.364	-0.496	(0)
FeHSO4+2	1.205e-25	9.053e-26	-24.919	-25.043	-0.124	(0)
FeCl3	8.083e-28	8.091e-28	-27.092	-27.092	0.000	(0)
Fe3(OH)4+5	7.638e-29	1.281e-29	-28.117	-28.892	-0.775	(0)
H(0)	0.000e+00					
H2	0.000e+00	0.000e+00	-46.125	-46.125	0.000	28.62
K	9.232e-05					
K+	9.220e-05	8.578e-05	-4.035	-4.067	-0.031	8.64
KSO4-	1.193e-07	1.113e-07	-6.923	-6.954	-0.030	33.78

Mg	1.592e-04					
Mg+2	1.516e-04	1.150e-04	-3.819	-3.939	-0.120	-21.32
MgSO4	4.543e-06	4.548e-06	-5.343	-5.342	0.000	5.37
MgHCO3+	2.623e-06	2.442e-06	-5.581	-5.612	-0.031	5.14
MgCO3	4.769e-07	4.774e-07	-6.322	-6.321	0.000	-17.08
MgOH+	1.234e-08	1.152e-08	-7.909	-7.938	-0.030	(0)
Mn(2)	9.101e-09					
Mn+2	6.188e-09	4.699e-09	-8.208	-8.328	-0.120	-20.58
MnCO3	1.907e-09	1.909e-09	-8.720	-8.719	0.000	(0)
MnHCO3+	8.439e-10	7.867e-10	-9.074	-9.104	-0.030	(0)
MnSO4	1.514e-10	1.516e-10	-9.820	-9.819	0.000	28.02
MnCl+	7.418e-12	6.915e-12	-11.130	-11.160	-0.030	-6.27
MnOH+	3.935e-12	3.668e-12	-11.405	-11.436	-0.030	(0)
MnCl2	1.089e-15	1.090e-15	-14.963	-14.962	0.000	101.08
MnCl3-	1.164e-19	1.085e-19	-18.934	-18.965	-0.030	43.76
Mn(OH)3-	3.242e-20	3.022e-20	-19.489	-19.520	-0.030	(0)
Mn(3)	2.314e-21					
Mn+3	2.314e-21	1.289e-21	-20.636	-20.890	-0.254	(0)
Na	1.176e-03					
Na+	1.174e-03	1.094e-03	-2.930	-2.961	-0.031	-2.08
NaHCO3	1.228e-06	1.229e-06	-5.911	-5.910	0.000	1.80
NaSO4-	1.225e-06	1.143e-06	-5.912	-5.942	-0.030	14.24
NaCO3-	6.445e-08	6.000e-08	-7.191	-7.222	-0.031	-2.23
NaOH	3.504e-20	3.508e-20	-19.455	-19.455	0.000	(0)
O(0)	4.391e-04					
O2	2.195e-04	2.198e-04	-3.658	-3.658	0.000	29.45
Pb	1.289e-07					
PbCO3	1.205e-07	1.206e-07	-6.919	-6.919	0.000	(0)
PbHCO3+	2.176e-09	2.026e-09	-8.662	-8.693	-0.031	(0)
PbOH+	2.105e-09	1.960e-09	-8.677	-8.708	-0.031	(0)
Pb(CO3)2-2	2.062e-09	1.549e-09	-8.686	-8.810	-0.124	(0)
Pb+2	1.807e-09	1.358e-09	-8.743	-8.867	-0.124	-15.35
PbSO4	1.704e-10	1.706e-10	-9.768	-9.768	0.000	(0)
Pb(OH)2	5.639e-11	5.645e-11	-10.249	-10.248	0.000	(0)
PbCl+	1.599e-11	1.489e-11	-10.796	-10.827	-0.031	7.52
Pb(SO4)2-2	2.662e-13	2.001e-13	-12.575	-12.699	-0.124	(0)
Pb(OH)3-	5.153e-14	4.798e-14	-13.288	-13.319	-0.031	(0)
PbCl2	1.044e-14	1.045e-14	-13.981	-13.981	0.000	33.97
Pb2OH+3	1.133e-16	5.957e-17	-15.946	-16.225	-0.279	(0)
Pb(OH)4-2	1.083e-17	8.138e-18	-16.965	-17.090	-0.124	(0)
PbCl3-	3.011e-18	2.804e-18	-17.521	-17.552	-0.031	64.46
Pb3(OH)4+2	2.558e-20	1.923e-20	-19.592	-19.716	-0.124	(0)
PbCl4-2	5.930e-22	4.456e-22	-21.227	-21.351	-0.124	99.42
Pb(HS)2	0.000e+00	0.000e+00	-290.283	-290.283	0.000	(0)
Pb(HS)3-	0.000e+00	0.000e+00	-437.295	-437.326	-0.031	(0)
S(-2)	0.000e+00					
CdHS+	0.000e+00	0.000e+00	-146.824	-146.855	-0.031	(0)
HS-	0.000e+00	0.000e+00	-148.311	-148.343	-0.031	20.01
H2S	0.000e+00	0.000e+00	-149.119	-149.119	0.000	37.12
S-2	0.000e+00	0.000e+00	-153.595	-153.717	-0.122	(0)
Cd(HS)2	0.000e+00	0.000e+00	-288.839	-288.838	0.000	(0)
Pb(HS)2	0.000e+00	0.000e+00	-290.283	-290.283	0.000	(0)
Fe(HS)2	0.000e+00	0.000e+00	-305.993	-305.993	0.000	(0)
Cu(HS)3-	0.000e+00	0.000e+00	-427.571	-427.602	-0.031	(0)
Cd(HS)3-	0.000e+00	0.000e+00	-434.970	-435.001	-0.031	(0)
Pb(HS)3-	0.000e+00	0.000e+00	-437.295	-437.326	-0.031	(0)
Fe(HS)3-	0.000e+00	0.000e+00	-452.267	-452.298	-0.031	(0)
Cd(HS)4-2	0.000e+00	0.000e+00	-581.030	-581.154	-0.124	(0)
S(6)	3.269e-04					
SO4-2	2.960e-04	2.235e-04	-3.529	-3.651	-0.122	12.90
CaSO4	2.493e-05	2.496e-05	-4.603	-4.603	0.000	7.04
MgSO4	4.543e-06	4.548e-06	-5.343	-5.342	0.000	5.37
NaSO4-	1.225e-06	1.143e-06	-5.912	-5.942	-0.030	14.24
KSO4-	1.193e-07	1.113e-07	-6.923	-6.954	-0.030	33.78
BaSO4	3.914e-08	3.918e-08	-7.407	-7.407	0.000	(0)
HSO4-	2.530e-10	2.355e-10	-9.597	-9.628	-0.031	39.43
PbSO4	1.704e-10	1.706e-10	-9.768	-9.768	0.000	(0)
MnSO4	1.514e-10	1.516e-10	-9.820	-9.819	0.000	28.02

CuSO4	1.420e-10	1.422e-10	-9.848	-9.847	0.000	11.55
CdSO4	1.251e-10	1.253e-10	-9.903	-9.902	0.000	84.16
CaHSO4+	2.073e-12	1.931e-12	-11.683	-11.714	-0.031	(0)
Cd(SO4)2-2	4.366e-13	3.281e-13	-12.360	-12.484	-0.124	-113.88
Pb(SO4)2-2	2.662e-13	2.001e-13	-12.575	-12.699	-0.124	(0)
AlSO4+	4.127e-14	3.845e-14	-13.384	-13.415	-0.031	(0)
Al(SO4)2-	2.772e-16	2.583e-16	-15.557	-15.588	-0.031	(0)
FeSO4+	2.626e-18	2.448e-18	-17.581	-17.611	-0.030	(0)
FeSO4	1.800e-20	1.801e-20	-19.745	-19.744	0.000	31.95
Fe(SO4)2-	1.232e-20	1.147e-20	-19.909	-19.940	-0.031	(0)
AlHSO4+2	5.667e-23	4.259e-23	-22.247	-22.371	-0.124	(0)
FeHSO4+2	1.205e-25	9.053e-26	-24.919	-25.043	-0.124	(0)
FeHSO4+	1.684e-27	1.568e-27	-26.774	-26.805	-0.031	(0)
Si	1.954e-04					
H4SiO4	1.939e-04	1.941e-04	-3.712	-3.712	0.000	53.11
H3SiO4-	1.536e-06	1.430e-06	-5.814	-5.845	-0.031	27.65
H2SiO4-2	4.579e-12	3.466e-12	-11.339	-11.460	-0.121	(0)

----------Saturation indices----------

Phase	SI**	log IAP	log K(287 K, 1 atm)	
Al(OH)3(a)	-1.11	10.41	11.51	Al(OH)3
Albite	-0.93	-19.63	-18.70	NaAlSi3O8
Alunite	-3.71	-3.76	-0.05	KAl3(SO4)2(OH)6
Anglesite	-4.67	-12.52	-7.85	PbSO4
Anhydrite	-2.65	-6.82	-4.17	CaSO4
Anorthite	-1.63	-21.65	-20.03	CaAl2Si2O8
Aragonite	-0.18	-8.46	-8.28	CaCO3
Barite	0.05	-10.11	-10.15	BaSO4
Ca-Montmorillonite	3.82	-42.77	-46.60	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	-0.03	-8.46	-8.43	CaCO3
Cd(OH)2	-6.59	7.06	13.65	Cd(OH)2
CdSiO3	-6.16	3.34	9.51	CdSiO3
CdSO4	-12.63	-12.33	0.30	CdSO4
Cerrusite	-0.90	-14.16	-13.26	PbCO3
CH4(g)	-147.66	-150.41	-2.75	CH4
Chalcedony	-0.03	-3.71	-3.68	SiO2
Chlorite(14A)	-3.78	68.67	72.45	Mg5Al2Si3O10(OH)8
Chrysotile	-5.58	27.98	33.55	Mg3Si2O5(OH)4
CO2(g)	-2.84	-4.17	-1.33	CO2
Dolomite	-0.85	-17.69	-16.84	CaMg(CO3)2
Fe(OH)3(a)	0.82	5.71	4.89	Fe(OH)3
FeS(ppt)	-154.82	-158.73	-3.92	FeS
Gibbsite	1.68	10.41	8.72	Al(OH)3
Goethite	6.32	5.71	-0.61	FeOOH
Gypsum	-2.23	-6.82	-4.59	CaSO4:2H2O
H2(g)	-43.05	-46.12	-3.07	H2
H2O(g)	-1.78	-0.00	1.78	H2O
H2S(g)	-148.19	-156.21	-8.02	H2S
Halite	-7.96	-6.40	1.56	NaCl
Hausmannite	1.52	65.25	63.73	Mn3O4
Hematite	14.61	11.43	-3.18	Fe2O3
Illite	3.16	-38.58	-41.74	K0.6Mg0.25Al2.3Si3.5O10(OH)2
Jarosite-K	-9.47	-17.84	-8.37	KFe3(SO4)2(OH)6
K-feldspar	0.67	-20.73	-21.40	KAlSi3O8
K-mica	9.59	23.88	14.30	KAl3Si3O10(OH)2
Kaolinite	5.00	13.39	8.38	Al2Si2O5(OH)4
Mackinawite	-154.08	-158.73	-4.65	FeS
Manganite	3.58	28.92	25.34	MnOOH
Melanterite	-19.56	-21.91	-2.35	FeSO4:7H2O
O2(g)	-0.85	-3.66	-2.81	O2
Otavite	-1.87	-13.97	-12.10	CdCO3
Pb(OH)2	-1.65	6.87	8.53	Pb(OH)2
Pyrite	-253.14	-271.92	-18.78	FeS2
Pyrochroite	-7.79	7.41	15.20	Mn(OH)2
Pyrolusite	7.30	50.43	43.13	MnO2:H2O
Quartz	0.43	-3.71	-4.14	SiO2

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  Rhodochrosite    -2.53    -13.62  -11.09  MnCO3
  Sepiolite        -3.58     12.46   16.05  Mg2Si3O7.5OH:3H2O
  Sepiolite(d)     -6.20     12.46   18.66  Mg2Si3O7.5OH:3H2O
  Siderite        -12.72    -23.55  -10.82  FeCO3
  SiO2(a)          -0.91     -3.71   -2.80  SiO2
  Sulfur         -111.23   -106.10    5.14  S
  Sylvite          -8.35     -7.51    0.85  KCl
  Talc             -2.09     20.55   22.64  Mg3Si4O10(OH)2
  Witherite        -3.15    -11.75   -8.60  BaCO3

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
  For ideal gases, phi = 1.

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End of simulation.
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Reading input data for simulation 4.
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End of Run after 0.24 Seconds.
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