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# INVESTIGATION OF THE IRON OXIDATION KINETICS

### IN MANTUA RESERVOIR

by

Scott H. Lathen

A thesis submitted to the faculty of

Brigham Young University

in partial fulfillment of the requirements for the degree of

Master of Science

Department of Civil and Environmental Engineering

Brigham Young University

August 2007

### BRIGHAM YOUNG UNIVERSITY

### GRADUATE COMMITTEE APPROVAL

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#### ABSTRACT

# INVESTIGATION OF THE IRON OXIDATION KINETICS IN MANTUA RESERVOIR

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Irrigation of the municipal cemetery in Brigham City, Utah resulted in stained headstones in 2001 and 2002. The water used in the irrigation came from Mantua reservoir, a medium sized impoundment situated near the mouth of Box Elder Canyon. In order for Brigham City to establish a city wide secondary pressurized irrigation system using water from Mantua reservoir, the cause and the source of staining problem must be determined. Previous research (Wallace 2006) determined that the source of the staining was the reduction of iron found in Mantua Reservoir sediments that occurred when seasonal variations in the reservoir caused anaerobic conditions. The reduced iron then dissolved in the water and was used in the irrigation system, causing re-oxidation of the iron. The oxidized iron then precipitated out on the headstones causing the staining. The

purpose of this investigation is to determine the iron oxidation kinetics after the reaeration of the water which will help determine appropriate mitigation methods. A secondary purpose is to confirm the Mantua reservoir's capacity to become anaerobic, resulting in the conditions which cause staining.

Using laboratory investigations and computer modeling, I determined that on reaeration, fifty percent of the dissolved iron in the water precipitates in five hours. Using first-order kinetics to model this process, I found the rate constant of the kinetic reaction to be 0.0029 min<sup>-1</sup>. Fitting a geochemical computer model of the iron oxidation kinetics in Mantua reservoir, which uses a higher-order kinetics model to better model this process, to experimental kinetic data yielded a rate constant of  $4x10^{13}/atm x min$ .

I also recreated the staining process in the laboratory using concrete. This was successful and provided visual evidence that the iron precipitates out of the water and stained the concrete within a couple of hours of application. Field data collected from Mantua reservoir showed that the dissolved oxygen concentration in the reservoir drops regularly below levels consistent with equilibrium to the atmosphere. While my field measurements did not record anaerobic conditions, based on the patterns shown, this study shows that it would be possible for anaerobic conditions to occur during warmer weather.

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### **1** Introduction

Brigham City, Utah installed a pressurized irrigation system to provide more effective water use and make irrigation more efficient. The system was restricted to just irrigating the city cemetery in the initial installation, though expansion to the rest of the City was planned. The system ran without serious problems until 2001, when workers found the headstones in the municipal cemetery were stained a dark reddish brown (Bigelow 2002). Ferric iron (Fe<sup>3+</sup>) had precipitated from the irrigation water, caused the staining on the headstones, and is the source of the red color of the stain (Wallace 2006). The water used in the pressurized irrigation system comes from Mantua Reservoir.

After the first appearance of the staining, the city shock treated the pipeline with bactericides in order to eliminate a biofilm observed to be lining the pipes. At this time, it was thought that the biofilm was the main factor causing the staining. The city also introduced iron and manganese sequestering agents, as well as chlorinated the water in an effort to prevent a recurrence of the staining. The staining did not occur during the remainder of that watering season, however the staining did return during the 2002 irrigation season despite the continued water treatments initiated the previous year.

Due to the continued staining from the system, Brigham City refrained from using Mantua water in the irrigation system and has switched to culinary water (Bigelow 2002).

Figure 1-1 is a photograph taken from the Brigham City cemetery sexton's report on the staining.



Figure 1-1: Headstone staining (Wood 2002)

The staining has not occurred in a predictable pattern or at a constant frequency and it has been difficult to establish common links between the staining events, this caused significant difficulty in determining the source and cause of the staining so they can use the Mantua water in the pressurized irrigation system and expand the irrigation system beyond the cemetery.

In 2005, Brigham City initiated a feasibility study to explore the possibility of creating a city wide pressurized irrigation system. Mantua Reservoir was identified as one potential and preferred source for the irrigation water (Bigelow 2005). This proposed expansion is not feasible using water from Mantua Reservoir until the threat of iron staining is removed. The city wants to understand the source of the staining, the mechanisms and situations that cause staining, and develop potential measures that can be taken to eliminate or minimize the problem.

#### 1.1 Mantua Reservoir Background

Mantua Reservoir, shown in Figure 1.2, is a medium-sized reservoir located at the top of Box Elder Canyon just east of Brigham City. Table 1-1 summarizes the significant attributes of Mantua Reservoir (Loveless *et al* 1997).

Elevation (ft):	5159
Surface Area	554
Watershed Area	5559
Capacity (acre-	10450
Mean Depth (ft):	14
Max Depth (ft):	20
Length (miles):	1.12
Width (miles):	1.02
Shoreline (miles):	2.1

Mantua Reservoir is a shallow reservoir that has a fairly large surface area. These two characteristics make the water unusually warm, exceeding the state guidelines of 20°C for a cold water fishery, promoting the growth of a myriad of aquatic life (Loveless *et al* 1997). Mantua also has a high loading of nutrients including phosphorus loadings that usually exceed regulations. The reservoir, shown in Figure 1-2, supports large blooms of blue-green algae and the production of macrophytes. The large quantity of aquatic organisms contributes to a low amount of dissolved oxygen (DO) in the system (Loveless *et al* 1997). The lake's beneficial use classification is 3A, a cold water fishery, 2B, for recreational use, and 4, protected for agricultural irrigation uses (Utah Department of Environmental Quality 2000).



Figure 1-2 : Mantua Reservoir

In the course of the Clean Lakes Study (Loveless *et al* 1997) it was observed that during the period from May to September, the DO concentration within one meter of the reservoir bottom was depressed below acceptable levels which were 3.0 mg/L. The DO conditions improved between July 18<sup>th</sup> and August 10<sup>th</sup> because of increased wind action, resulting in better mixing in the reservoir, mixing the aerated surface water with the lower waters. The low DO concentrations in the summer resulted from the hot stagnant conditions, decomposition of organic matter, and photosynthesis by aquatic vegetation (Loveless *et al* 1997).

The area surrounding the reservoir contributes to the characteristics in Mantua Reservoir that result in low DO. The Mantua Fish Hatchery is located at the head waters of Maple Creek, a major contributor to Mantua Reservoir. The hatchery is a major point source for total phosphorus loading to the reservoir which supports the high level of biological activity observed. Also of significance to this study is the composition of the sediments surrounding the reservoir and forming the bed of the reservoir. These sediments have a very high quantity of iron (III) minerals in the soil. Loveless *et al* (1997) gives the iron concentration in the lake bed sediments as 16,600 and 13,300 (mg/kg) respectively in the North and South arms of the reservoir. Wallace (2006) found the concentration of ferric iron in the reservoir sediments to be 16,500 mg/kg dry weight in sediment samples taken near the outlet and dam.

Big Creek is the outlet for Mantua Reservoir and has an average flow of 21 cubic feet per second. Brigham City captures Big Creek at the reservoir outlet and pipes the water into the city for power and irrigation uses. The head difference between the

reservoir and the city also allows the water to be used as a power generating source (Loveless *et al* 1997).

Previous research by Wallace (2006) determined that the iron found in the sediments of Mantua Reservoir is responsible for the staining of the Brigham City. The research concluded that when conditions cause the hypolimnion of the reservoir to become anaerobic, the ferric iron in the sediments is reduced to ferrous iron. Ferrous iron has a solubility constant sixteen orders of magnitude higher (Sawyer et al 2003) than ferric iron and therefore readily dissolves into the reservoir water. This dissolution process is catalyzed by biological activity which greatly increases the rate at which the iron dissolves. The iron-rich water is then taken into the reservoir outlet and piped to Brigham City in a closed system that is not re-aerated. When the iron saturated water leaves the Brigham City irrigation system and is sprayed onto the cemetery lawn, the water is re-aerated causing the ferrous iron to oxidize to ferric iron. At this point, the water becomes over saturated with respect to iron which then precipitates onto the headstones of the cemetery causing the observed staining (Wallace 2006). The reason the observed staining occurred intermittently was because the exact conditions which would cause the reservoir to go anaerobic are not common. These conditions occur at night during low-water, high-temperature, and low-wind conditions. Under these conditions degradation of biological matter in the reservoir uses the available oxygen and under these conditions there is no mechanism for re-aeration of the hypolimnion waters at the bottom of the reservoir.

#### 1.2 Objectives

The objective of my research is to determine the kinetics of the oxidation of ferrous iron to ferric iron and the subsequent precipitation of the ferric hydroxides, the source of the staining in Brigham City. Understanding the kinetics of this reaction will allow various treatment and mitigation alternatives to be evaluated. Previous research (Wallace 2006) determined that iron in the reservoir water does undergo reduction and oxidation based on the dissolved oxygen conditions in the water and is potentially catalyzed by microorganisms, speeding up the dissolution of the iron from the sediments to the water. The knowledge of the iron chemistry which occurs and causes this problem allows Brigham City to focus on remediation of the iron at the source. Modeling the kinetics of the oxidation reaction will allow Brigham City to choose the most effective treatment method and aid in design of a chosen treatment system.

In order to determine the reaction kinetics, I have used both experimental procedures and theoretical models. The experimental approach involved taking water and sediment samples from Mantua and allowing them to go anaerobic. The anaerobic conditions forced the reduction of ferric iron found in the sediments allowing the newly formed ferrous iron to dissolve in the water. I then re-aerated the water, causing the oxidation of the ferrous iron back to the ferric state, and recorded the amount of ferrous iron remaining after established time periods had elapsed. By repeating the experiment at various times, I generated a rate curve which describes the iron oxidation kinetics for the combination of Mantua Reservoir water and sediments.

In an effort to confirm the findings of Wallace (2006) who determined the staining mechanism, I recorded the reservoir DO levels over an extended period of time

to determine if DO levels near the bottom of the reservoir were significantly depleted at night. Also using the water and sediment samples collected from the reservoir I have replicated the staining seen in the Brigham City cemetery.

I developed the theoretical geochemical model using PHREEQC, developed by Parkhurst and Appelo (1999), to model the oxidation kinetics. The parameters used to create and define this model were taken from the Clean Lakes Study (Loveless *et al* 1997) performed on Mantua Reservoir. After the development of a preliminary model based on these data, I used the experimental data obtained from the laboratory procedures using Mantua Reservoir water and sediments to refine the model to fit the measurements I had which characterize Mantua Reservoir. A model of the iron oxidation kinetics allows a number of different scenarios to be evaluated and recommendations can be made to determine the treatment options available to Brigham City.

### 2 Chemistry

#### 2.1 Chemical Conditions of Mantua Reservoir

Previous studies conducted on Mantua Reservoir (Loveless *et al* 1997 and Wallace 2006) determined the general geochemistry that governs the reservoir. The Clean Lakes Study (Loveless *et al* 1997) described the nutrients, metals, and chemicals found in the reservoir, the inlets to the reservoir, and in the sediments forming the lake bed. Of particular interest to my research is the amount of iron that was found in the sediment and water of the reservoir and the DO conditions of Mantua. The study found that iron levels in the reservoir water averaged less than 20  $\mu$ g/L over the course of the study. However, the iron levels in the lake bed sediments were quite high in both the north and south arms of the reservoir with measurements of 16,600 mg/Kg and 13,300 mg/Kg respectively (Loveless *et al* 1997).

The Clean Lakes Study (Loveless *et al* 1997) also recorded the DO in Mantua Reservoir. The DO levels found in this study were a source of extra concern during the summer months, May through September, because they were low. This is the same time of the year as when the cemetery staining occurred. During these months the DO was measured to be less than 3.0 mg/L within one meter of the reservoir bottom. The water above one meter from the bottom generally had measured DO levels within acceptable parameters. Exceptions occurred on several days, most notably July 18<sup>th</sup>, when low DO levels were measured farther from the reservoir bottom. On July 18<sup>th</sup> the DO was measured at only 1.0 mg/L two meters from the bottom. This indicates that under some conditions, the DO levels in the bottom of the reservoir could become anaerobic.

Research by Wallace (2006) concluded that low DO, especially completely anaerobic conditions, would cause the iron in the sediments to reduce to the ferrous state and dissolve in the reservoir water. Iron reduction is a geochemical process that is probably accomplished by the microorganisms in the water using iron (III) as the terminal electron acceptor instead of oxygen (Sawyer et al 2003). This biological process also speeds up the iron dissolution. Ferrous iron ( $Fe^{2+}$ ) has a solubility product (ksp) that is fifteen orders of magnitude higher than ferric iron allowing the ferrous iron to dissolve into the reservoir water at significantly higher amounts that are possible under aerated conditions (Sawyer et al. 2003). Once the anaerobic reservoir water, with the dissolved ferrous iron, is re-oxygenated, such as through the action of being sprayed out of a sprinkler system, the iron (II) oxidizes to form the insoluble iron (III) which is oversaturated with respect to iron. The excess iron then precipitates as ferric hydroxide compounds causing the staining observed in the cemetery (Wallace 2006). In order to characterize and replicate these natural conditions Wallace (2006) collected water and sediment samples from Mantua. These samples were placed in BOD bottles, allowing the water to become anaerobic. The bottles were opened and DO was measured to confirm anaerobic conditions. At this point the water was stirred in order to accomplish aeration. At each stage, the original water, the anaerobic water in contact with the sediments, and the re-aerated water, the concentration of ferrous iron in solution was measured using the phenanthroline method and a spectrophotometer. Figure 2-1 is a bar

chart showing the concentration of ferrous iron in the water under the various DO conditions measured in this study to characterize the processes observed using water and sediment collected at Mantua reservoir.



Figure 2-1: March 31st results (Wallace 2006)

The water under anaerobic conditions contains a significantly higher concentration of ferrous iron, this represents the conditions that could occur during warm, wind-free summer nights at Mantua. Upon re-oxygenation the ferrous iron concentration in solution drops from almost 7 ppm to about 3.5 ppm, the iron is precipitated from solution. This drop in iron concentrations from the anaerobic water conditions to the reaerated water conditions is attributed to the oxidation of the ferrous iron creating insoluble ferric iron that precipitates out of the reservoir water and causes the problematic staining on the headstones (Wallace 2006).

#### 2.2 Iron Oxidation Kinetics

The research of Wallace (2006) demonstrated that the mechanism for the headstone staining was the change in the aerobic condition of the water and the subsequent reduction and oxidation of the iron found in the lake bed sediments. In addition to knowing the staining mechanism, it is important to know the kinetics of the reaction in order to provide treatment recommendations.

Only minor changes in environmental conditions are necessary to initiate the oxidation or reduction of iron in natural systems (O'Neil 1985). The mixing of oxygen, at even small amounts, with the ferrous iron oxidizes the iron, forming the insoluble ferric iron ( $Fe^{3+}$ ) which then will precipitate out of the water and cause staining (Sawyer et. al. 2003). Equation 2-1 is the reaction describing the oxidation of ferrous iron and the precipitation of ferric hydroxides:

$$4Fe^{2^+} + O_2 + 10H_2O \leftrightarrow 4Fe(OH)_{3(s)} \downarrow + 8H^+$$
(2-1)

Iron oxidation kinetics has been vigorously studied resulting in established mathematical models used to predict the rate of iron oxidation in various systems. Singer and Stumm (1970) investigated iron oxidation kinetics, determining that the rate of oxidation follows a predictable model. Their research yielded the widely accepted equation (equation 2-2) describing the kinetics of ferrous iron oxidation.

$$\frac{-d[Fe^{2+}]}{dt} = k[Fe^{2+}][OH^{-}]^2 Po_2$$
(2-2)

 $Po_2$  is the partial pressure of the atmospheric oxygen exerted on the water surface and can be replaced with the DO concentration in the water (Stumm and Lee 1961). The rate constant, *k*, varies with the experimental method used to determine it. Equation 2-2 is first order with respect to the ferrous iron concentrations and second order with respect to the concentration of the hydroxyl ions. As a result, the greater the pH of the water, the faster the ferric iron forms and can precipitate (Houben 2004). Table 2-1 summarizes different values used for the rate constant.

Rate Constant <sup>1</sup> k (1/mol <sup>3</sup> x min)	Temperature (°C)	Reference
0.8-1.7x10 <sup>16</sup>	10	Davison and Seed (1983)
1.4x10 <sup>16</sup>	25	Tamura et al. (1976)
0.7x10 <sup>16</sup>	10	Millero et al. (1987)
1.7(±0.4)x10 <sup>16</sup>	10	Laxen and Sholkovitz (1981)
6.0x10 <sup>16</sup>	25	Stumm and Morgan (1996)

Table 2-1: Rate Constants for Iron Oxidation<sup>2</sup>

<sup>1</sup> rate constant for concentration of dissolved oxygen

<sup>2</sup> Modified from Houben (2004)

Equation 2-2 can be arraigned to be a function of pH instead of the hydroxyl ion concentrations (Houben 2004). This results in equation 2-3 which shows the oxidation rate as a function of both the DO concentration and the pH (or  $[H^+]$ ):

$$\frac{-d[Fe^{2+}]}{dt} = k[Fe^{2+}][H^+]^{-2}[O_{2(aq)}]$$
(2-3)

where *k* is the kinetic rate constant,  $[Fe^{2+}]$  is the concentration of the ferrous iron dissolved in the water,  $[H^+]$  is the concentration of the hydrogen ions, and  $[O_{2(aq)}]$  is the concentration of DO in the aqueous solution. At pH values less than 3.5, the rate of iron oxidation is independent of the pH and that term is dropped from the equation. When this term is dropped, the rate constant increases to  $1.0 \times 10^{-7}$  (Singer and Stumm 1970).

Since the oxidation of ferrous iron is proportional to the concentration of ferrous iron in the reservoir, when other parameters are held constant, first-order kinetics can be used to determine the experimental rate constant (k). Equation 2-4 is the equation that describes these first-order kinetics (Sawyer *et al* 2003).

$$C = C_0 e^{-kt} \tag{2-4}$$

where *C* is the final concentration of the substance,  $C_0$  is the initial concentration at t = 0, *t* is the time that the reaction proceeds, and *k* is the kinetic rate constant for the reaction. It should be noted that while all these equations use *k* as the rate constant, it is different for each equation used.

#### 2.3 Factors Affecting Iron Oxidation Kinetics

A number of factors can influence the rate of ferrous iron oxidation (Liang 1993). Various environmental conditions, the presence of other ions, and the presence of iron oxidizing bacteria can all increase the rate of oxidation. Of the possible environmental factors, an increase in pH has the most dramatic effect on the kinetics of the system. A unit increase in the pH will result in a 100-fold increase in the oxidation rate of the ferrous iron (Morgan and Stumm 1996). Though less dramatic, a 15 degree Celsius change in the system, for a constant pH, will result in a 10-fold increase in the oxidation rate (Morgan and Stumm 1996). At high pH levels, greater than 7, the oxidation of the soluble ferrous iron in the system can happen in just minutes (Appelo and Parkhurst 2005). The increased oxidation rate resulting from a higher pH is a consequence of enhanced electron-transfer capacity (Houben 2004).

The presence of other metal ions can also have a catalytic effect on the oxidation of ferrous iron; particularly  $Cu^{2+}$  and  $Co^{2+}$  in trace amounts increase the reaction rate (Morgan and Stumm 1996). Other anions that form complexes with iron will also speed up the reaction (Morgan and Stumm 1996). Of particular note, when ferric iron is added to the water, it acts as a catalyst for the ferrous to ferric iron reaction (Tamura *et al* 1976). As a result, the more ferrous iron oxidized to the ferric state, the faster the reaction proceeds. Tamura *et al* (1976) proved that the catalytic effect of ferric iron happens as the ferrous iron in solution sorbs onto the suspended ferric iron particles. The ferrous iron is then oxidized on the surface of the ferric iron particles. Rising pH linearly increases the sorption of ferrous iron due to the higher amount of negative surface charge of the oxide. The increased rate of oxidation from the inclusion of ferric iron in the system leads to a new kinetic model based on equations 2-2 and 2-3 (Tamura *et al* 1976). Equation 2-5 is the revised kinetic model:

$$\frac{-d[Fe^{2+}]}{dt} = k_1 [Fe^{2+}] [H^+]^{-2} [O_{2(aq)}] + k_2 [Fe^{3+}] [Fe^{2+}] [H^+]^{-2} [O_{2(aq)}]$$
(2-5)

where  $k_2$  is the product of the equilibrium constant for the sorption of Fe<sup>2+</sup> onto ferric oxide and the rate constant of the oxidation at the surface. The value of this constant is given as  $1.71 \times 10^{-5}$  mol/min (Tamura *et al* 1976). Equation 2-5 indicates that the pH has a more significant impact on the homogenous portion of the equation than on the heterogeneous part. Therefore the effect of ferric iron on the reaction rate is more important at lower pH levels. The catalytic effect of ferric iron is significant only when the concentrations of ferrous iron is greater than 3 mg/L otherwise there is insufficient catalytic surface to greatly impact the kinetics (Tamura *et al* 1976). This implies that once precipitation and staining start, it will proceed rapidly.

In addition to metal ions and physical environmental conditions, the presence of iron oxidizing bacteria will significantly increase the rate of the reaction (Okereke and Stevens 1991), just as iron-reducing bacteria can significantly increase the dissolution rate from the sediments (Wallace 2006). The presence of microbes can accelerate the reaction rate by a factor of  $10^6$  (Singer and Stumm 1970). *Thiobacillus ferrooxidans* are the bacteria most responsible for the oxidation of ferrous iron in low DO conditions. *T. ferrooxidans* are acidophilic chemolithotrophs that will increase the oxidation rate of Fe<sup>2+</sup> when the pH values in the water fall below 3.5 (Okereke and Stevens 1991). The effect of the microbes on the kinetics of the reaction varies greatly depending on the environmental conditions present. Included in the variables which can affect the system is the actual concentration of the bacteria present in the system. An increase in the concentration of *T. ferrooxidans* results in an increase in the rate of the reaction. Equation 2-6 describes the oxidation rate of ferrous iron based on the bacterial

concentration, the ferrous iron concentration, and the temperature of the system (Okereke and Stevens 1991):

$$Y = 0.68(B) + 0.02(B)(T) + 1.8x10^{-4}(T^2) - 0.46(B^2) -5x10^{-5}(F)(T) - 1.2x10^{-3}(F)(B) - 0.22$$
(2-6)

where B is the bacterial cell concentration (mg/mL) and F is the ferrous iron concentration (millimolar) with T being the temperature in degrees Celsius (Okereke and Stevens 1991).
# **3** Methods and Experimental Procedures

#### **3.1** Sampling Methods and Locations

In order to determine the kinetic reaction coefficient (*k*) for iron oxidation, water and sediment samples were collected from Mantua Reservoir and used in laboratory procedures to determine the ferrous iron content of the reservoir water at various oxidation states. The water entering the irrigation system is the water of highest concern for this study. The reservoir outlet that supplies the irrigation system is located on the west side of the reservoir. The samples collected for this study were taken from a floating pier, also located on the west side of the reservoir, approximately 100 feet from the reservoir outlet. Figure 3-1 is an aerial photo of Mantua Reservoir. The floating pier (not visible in the figure) is located at the south west corner of the reservoir. The outlet is approximately 100 ft to the north from the pier, along the western shore of the reservoir.

I used a soil auger to remove samples of the reservoir bottom sediments. These samples were taken from the sediments beneath the floating pier. After collecting the sediment samples in buckets, the remainder of each bucket was filled with water collected from the surface of the reservoir. Surface water has low dissolved ferrous iron due to the aerobic conditions present at the water and air interface (Campbell 1989). After collection, the sediment and water samples were transported back to the laboratory for analysis.



Figure 3-1: Aerial view of Mantua Reservoir

The samples used in the laboratory procedures were collected on two separate occasions. The first sample set was taken on September 8, 2006 in the early afternoon. The second sampling date was on October 6, 2006 also in the early afternoon. The procedures used for collecting the samples were the same for both days.

## 3.2 Qualitative Procedures

The first experiments performed were qualitative methods to confirm the findings of Wallace *et al* (2006) that the change in oxidation state of iron found in the lake bed sediments would cause the observed staining by first dissolving then precipitating iron from the sediments. In order to accomplish this objective, samples of water and sediment from Mantua Reservoir were subjected to the same conditions that we believe are responsible for the staining and the results were documented.

To perform these experiments, first the sediment and water from Mantua Reservoir was transferred to a BOD bottle. The bottle was a standard 300 mL BOD bottle with 1.25 inches of sediment on the bottom and the remainder filled with reservoir water. The BOD bottle was sealed and placed in a dark cabinet, to prevent photosynthesis from generating oxygen. Prior to the transfer of the water and sediment to the BOD bottles, a 16 oz bottle of Sprite was added to the water in the 5 gallon bucket, in order to renew the food source for the microbes. This was necessary to compensate for the delay between the time the water was collected from the reservoir and when it was used in the laboratory procedures. During this time, the bacteria used all the available food initially present in the reservoir water.

After allowing the BOD bottles to sit in the cabinet for three days, to completely deplete the DO, the water was sprayed onto a concrete core sample using a pump, simulating the action of a sprinkler in the Brigham City Cemetery irrigation system. I photographed the concrete core samples immediately before spraying with the Mantua water and several times over the next day to compare the amount of visible staining. These results are presented in Section 5.2.

#### 3.3 DO Testing in Mantua Reservoir

Along with laboratory procedures to confirm the findings of Wallace (2006), we also deployed a sonde in Mantua Reservoir to record the fluctuation of DO levels in the reservoir. The purpose of the DO measurements was to prove that the oxygen state of the

reservoir fluctuates and that the DO levels will reach sufficiently low levels to allow the reduction of ferric iron to soluble ferrous iron (Sawyer *et al* 2003). Wallace (2006) established conditions which could cause staining, but did not confirm that these conditions occur in Mantua Reservoir, which was the goal of these measurements. The data obtained from the sonde was correlated with weather station data in order to prove the hypothesis that temperature and wind conditions (which provides mixing of the reservoir water) contribute to the depletion of oxygen in the lower layers of the reservoir and that under the right conditions, water at the bottom of Mantua Reservoir could become anaerobic, dissolving high levels of iron from the sediments.

I used a YSI 600 OMS (optical monitoring sensor) sonde with an additional DO probe. The sonde is internally powered and capable of storing up to 150,000 bits of data. The DO probe is a YSI 6150 Optical Dissolved Oxygen Sensor. Optical sensors do not require changing a membrane frequently in order to achieve accurate results (YSI Incorporated 2006). Prior to deployment, the sonde and accompanying DO probe were calibrated according to the procedures in the operating manual (YSI Incorporated 2006). The sonde was deployed by swimming underneath the floating pier and using 8 feet of rope to attach it to a brace on the underside of the pier. This positioned the sonde about 2 to 3 feet above the sediment. The sonde was not positioned lower in case the reservoir levels changed during the measuring period, lowering the dock and potentially having the sonde contact the sediments.

The probe was set to record for a period of thirty days starting on September 8<sup>th</sup>, 2006. The sonde took readings every 15 minutes over this time period. The parameters measured were time, temperature, DO concentration, resistivity, total dissolved solids

(TDS), and salinity. Of these parameters, the DO concentration and temperature were the only data used in this study. The probe was retrieved on October 8<sup>th</sup>, 2006 using a DO probe recovery device that I constructed using a broom and an old metal hanger. The data was uploaded from the sonde to a computer and analyzed using the software included with the probe. The results of these measurements and discussions are included in Section 5.1.

#### 3.4 Laboratory Procedures

In order to determine the iron oxidation kinetics of Mantua Reservoir I used the collected samples to determine the kinetics rate constant (k). The laboratory procedures involved forcing the water samples to go anaerobic while in contact with the sediments, re-aerating the samples, and simultaneously recording the concentration of ferrous iron remaining in the water during the re-aeration period. The following sub-sections detail the steps required to accomplish each phase of the laboratory procedures.

## 3.4.1 Anaerobic Conditions

After transporting the samples from Mantua Reservoir to the lab, they were kept stored in sealed buckets until there was sufficient time to conduct the experimental procedures. The samples collected on September 8<sup>th</sup>, 2006 (the day the probe was deployed) were run on October 21<sup>st</sup>, 2006. The delay between collecting the samples and running the experimental procedures necessitated the addition of a food source for the microbes in order for them to use the available oxygen in the water and aid in the oxidation and reduction processes. The food source added was a 16 oz. bottle of Sprite. The sample bucket, which included two inches of sediment, was then sealed and stored in

a dark refrigeration room at normal room temperature of about 20 degrees Celsius. The bucket and water samples were then left overnight to allow time for the microbes to use all of the DO in the water as well as oxygen in the headspace of the bucket. In order to confirm the anaerobic state of the Mantua water samples, a YSI model DO probe was used to confirm the DO oxygen state of the water, which for these tests was zero.

#### 3.4.2 Standards

To measure the concentration of ferrous iron in the Mantua water as it was reaerated, a set of standards was prepared with known concentrations of iron. These standards were used to create a calibration curve to quantify experimental results.

To create the calibration curve I needed to determine the iron concentration range needed to fit the experimental data. For each trial, conducted with samples gathered on different days, new standards and calibration curves were created. Wallace *et al* (2006) found the maximum concentration of iron to be slightly less than 7 ppm for the samples collected on March 31<sup>st</sup>, 2006 with the minimum being essentially 0 ppm within the ranges of the method used. As a result, the four points I used for the calibration curve were nominally 1 ppm, 2 ppm, 5 ppm, and 8 ppm, which provided a smooth curve and bracketed the iron concentration range I required.

The standards were created by dissolving ferric chloride (FeCl<sub>3</sub>) in de-ionized (DI) water in a 1000-mL volumetric flask. In order to achieve an iron concentration of 100 ppm, 0.495 grams of ferric chloride were dissolved in the DI water. This produced an iron concentration of 102.265 mg/L in the 1000 mL flask. This concentrated standard was then diluted to the desired concentrations necessary for the calibration curve by mixing 1, 2, 5, and 8 mL, respectively from the concentrated 100 ppm standard into a 100

mL volumetric flask and filling with DI water. The actual concentrations of the four points on the calibration curve are given in Table 3-1. The spreadsheet used to calculate the necessary iron concentrations for the points on the calibration curve and the calculations used is included in Appendix C.

Desired Concentration (ppm)	Actual Dilution (ppm)		
1	1.023		
2	2.045		
5	5.113		
8	8.181		

Table 3-1: Standards

The calibration curve was created by measuring the known iron standards concentrations using the same procedures that the iron concentrations in the Mantua samples were measured. First, ten mL from each of the four standard concentrations were placed in test vials that fit the spectrophotometer. A packet of FerroVer Iron Reagent was then added to each vial. The reagent is a phenanthroline based powder that dissolves and creates a colorimetric change in the sample, the strength of which varies based on the concentration of the iron present. Each standard was measured in the spectrophotometer at a wavelength of 510 nanometers, the necessary wavelength to accurately determine the iron concentration (APHA 1995). The amount of light absorbed by each standard was recorded and a calibration curve was created based on the absorbance and the associated concentration of iron. Normally the calibration curve would be piecewise linear, using each measured data point. However, for these data, the curve approximated a straight line. To make calculations simpler, a linear trend line was

fit to the calibration points creating a linear equation that determines iron concentration based on the absorbance of a sample. Figure 3-2 is the calibration curve created using the ferric chloride standards.



Figure 3-2: Iron standards calibration curve

#### 3.4.3 Re-aeration and Iron Measurement

To measure the experimental results, the anaerobic state of the Mantua water sample was first confirmed, and then the procedure used to measuring the iron concentration in the standards was followed to measure the iron concentration in the Mantua water. First the water in the sample bucket was decanted from the sediment by pouring it into a smaller container. Immediately upon opening the bucket of anaerobic water, a sample was removed and the iron was measured. This sample was an attempt to measure the amount of dissolved iron before any aeration. A mixer was then placed in this bucket to provide adequate re-oxygenation to the entire water sample. At specified times, a sample of the Mantua water was removed from the mixing bucket and filtered using a bottle top filter and a vacuum pump. The purpose of the filtration was to ensure that the ferric iron that had already precipitated was removed from the sample and measure only the remaining ferrous iron in the reservoir water. After the sample was filtered, two ten mL test vials were prepared with the FerroVer reagent. The absorbance or these two vials were then measured in the spectrophotometer at the required wavelength of 510 nanometers. The recorded absorbance for each sample was compared to the calibration curve in order to determine the concentration of ferrous iron in the water, which was averaged for the two samples taken. This process was repeated as quickly as possible, being constrained by the time required to filter each sample. The result was a kinetics curve relating time since re-aeration to the concentration of ferrous iron remaining in the water. From the kinetics curve, and using the first-order kinetics equation (equation 2-4), the rate constant for iron oxidation kinetics in Mantua Reservoir was determined. This is discussed more fully in Section 5.3.

# 4 Computer Modeling Procedures

#### 4.1 PHREEQC

To better understand the iron oxidation kinetics of Mantua Reservoir I created a computer model. The model allowed me to evaluate the kinetics of iron oxidation for any conditions that may be present at the reservoir, based on the kinetic models present. The parameters that can be adjusted in the model related to iron precipitation kinetics include the water temperature, pH, and the loading rates of the various nutrients and inorganic constituents. The current conditions of the water at Mantua reservoir could be used to setup the model and using the experimentally determined k, the kinetics for iron oxidation can be predicted under various conditions.

The program used to develop the model of Mantua Reservoir was PHREEQC. PHREEQC was developed by Parkhurst and Appelo for United States Geological Survey (USGS). The program was created to conduct low temperature aqueous geochemical calculations (Parkhurst and Appelo 1999). In this case low temperatures are those expected in the surface environment, in many geochemical applications, the reactions take place at high temperatures deep underground. The primary use of PHREEQC is as a speciation program to calculate saturation indices and the distribution of aqueous species. Kinetic reactions can also be modeled using an embedded Basic editor. The kinetic rate

expressions are written using Basic and then PHREEQC interprets the code and runs the kinetic calculations (Parkhurst and Appelo 1999).

#### 4.2 Mantua Model Development

To develop a model of the iron oxidation kinetics taking place in Mantua Reservoir water, I used example 9 of the PHREEQC models provided with the program which was created to conduct kinetic calculations for the oxidation of ferrous iron to ferric iron. Example 9 is titled "Kinetic Oxidation of Dissolved Ferrous Iron with Oxygen" (Parkhurst and Appelo 1999) and is included in Appendix B. I used this example model as the basis for the iron oxidation kinetics model developed for Mantua Reservoir.

Example 9 is used in the documentation to demonstrate the ability of PHREEQC to conduct kinetic calculations for the oxidation of  $Fe^{2+}$  to  $Fe^{3+}$  in water (Parkhurst and Appelo 1999). The rate equation, Equation 4-1, used in the model was adapted from Singer and Stumm (1970):

$$\frac{dm_{Fe^{2+}}}{dt} = -\left(2.91x10^{-9} + 1.33x10^{12}\,\alpha_{OH^-}^2 P_{O_2}\right)m_{Fe^{2+}} \tag{4-1}$$

where *t* equals the time in seconds,  $a_{OH}^2$  is the activity of the hydroxyl ion,  $m_{Fe2+}$  is the total molality of ferrous iron in solution, and  $P_{O2}$  is the partial pressure of the oxygen (Parkhurst and Appelo 1999). The kinetics rate equation is solved using a 4th- and 5th-order Runge-Kutta-Fehlberg algorithm that is embedded within PHREEQC. PHREEQC calculates equilibrium before starting a kinetic calculation and again when each kinetic

reaction increment is added. The model calculates equilibrium for all solution-species, and for all exchange, equilibrium-phase, solid-solutions, surface assemblages and gas phases that are defined. A check is performed to ensure that the difference between the fourth- and fifth-order estimates of the integrated rate over a time interval does not vary by more than a user-defined tolerance. Failure to achieve results within the user defined tolerances will automatically restart the integration with a smaller time interval (Parkhurst and Appelo 1999).

The model I created of Mantua reservoir was based on the example provided with the program. Like the example, the purpose of the Mantua model is to simulate the oxidation of ferrous iron to ferric iron using oxygen in a natural water system, however the two models use separate geochemical environments. The PHREEQC model of Mantua Reservoir is presented in Appendix B. Several changes were required to adapt the example model to reflect the conditions present at Mantua reservoir. The first section of the Mantua model, SOLUTION\_MASTER\_SPECIES and SOLUTION\_SPECIES, decouples the valence state of iron and defines the possible iron species found in the water (Parkhurst and Appelo 1999). This section of the code remained unchanged from the example in the Mantua model.

The next section of the model, starting with EQUILIBRIUM\_PHASES 3, defines the conditions at Mantua Reservoir and defines the species that have the potential to precipitate out of the water, in this case ferric hydroxide. This section is followed by the SOLUTION1 section which defines the concentrations, in mmol/kilograms of water (kgw), of the applicable constituents and the physical characteristics of the water; this section was modified to match measured conditions at Mantua. Of particular importance

is the concentration of ferrous iron in the water, also expressed in mmol/kgw. The EQUILIBRIUM PHASES 1 heading defines the partial pressure of atmospheric oxygen that serves to aerate the water and cause the oxidation of the ferrous iron. This value is the negative log of the partial pressure for oxygen in the atmosphere at 5000 feet of elevation for the Mantua model (Parkhurst and Appelo 1999).

The final section of the PHREEQC model code is the kinetics calculation. The RATES data block is used to define the kinetics rate equation (see equation 4-1) used in the model calculations. This is followed by the KINETICS data block which invokes the rate expression and defines the parameters, especially the time increments. The final section of the code defines the desired output form of the results. For the Mantua model, a graph is created showing the total concentrations of ferrous and ferric iron versus time was created (Parkhurst and Appelo 1999).

After developing a generic model for Mantua Reservoir which used the measured field environmental data, I refined the model by adjusting the rate constant to fit the observed kinetics data for the oxidation of ferrous iron that was measured in the laboratory. This required adjusting the rate constant in Equation 4-1 by an order of magnitude from the value used in the example model. This rate increase can be attributed to microorganisms catalyzing the reaction, a factor that is not considered in the rate constant provided in the example. Mantua has significant biological activity and the example problem did not consider biological activity.

# 5 Experimental and Modeling Results and Discussion

#### 5.1 Field Results

Field measurement of the conditions at Mantua Reservoir was used to support my work and verify previous work. The deployment of the DO probe at Mantua Reservoir to measure DO values over time, served to confirm that the anaerobic conditions necessary to support the conclusions of Wallace (2006) could occur in the field. Data was collected by the sonde every fifteen minutes over a four week period starting the beginning of September, 2006 and ending the first week of October, 2006. A sample of the raw data obtained by the sonde is included in Appendix A. Figure 5-1 is a plot of the DO concentration and the water temperature of Mantua Reservoir over the period tested.

As expected, the DO concentration increases with lower water temperatures. Water has a greater capacity to dissolve and store oxygen at colder temperatures (Sawyer *et al* 2003). Of particular interest for the purposes of this study was the variation in the DO. Large variations, up to 6 ppm, occurred over relatively short periods as seen by the large repetitive changes between 50 to 150 hours and 500 to 600 hours. For example, on September 11<sup>th</sup>, 2006 (75 hours), starting at around 2:00 pm, the DO concentration in the reservoir steadily dropped from about 8.0 mg/L to 3.62 mg/L at 5:30 pm on the same day. The corresponding water temperature at the time only dropped one-tenth of a degree Celsius (from 19.28 degrees to 19.18). Using weather station data obtained from a site in



Figure 5-1: DO and temp measurements

nearby Brigham City, the maximum wind velocity during this period peaked at 5 miles per hour (mph) at 5:30 pm and the corresponding temperature at this time was 82 degrees Fahrenheit (Utah Department of Air Quality 2006). Although Mantua Reservoir and Brigham City are only about 5 miles apart (Mantua Reservoir TMDL 2000), the reservoir is located within the sheltered Box Elder Canyon so the wind and temperature profiles could vary significantly between the two locations. Also there is a difference of 782 feet in elevation between the weather station and the reservoir that could result in different wind velocities and air temperature at the two locations. The data collected from Mantua Reservoir includes ten instances in the one-month period, like the one described above, where a sharp drop in the DO concentration occurred over a matter of a few hours. A number of factors could have significant effect on the data collected and the data might not reflect the exact conditions at the water-sediment interface. Wallace (2006) concluded the reduction of iron in the sediments under anaerobic conditions, and the subsequent dissolution of the ferrous iron into the reservoir water, occurred immediately above the sediments at the bottom of the lake. The DO probe was deployed about two feet off the lake bottom for fear of dropping reservoir water levels, sinking the sonde into the sediments. At a greater depth, the DO concentration most likely drops more during the calm periods than the values measured as there is less mixing and diffusion of the oxygen from the atmosphere (Loveless *et al* 1997).

Another important consideration is the time period when the sonde was deployed. The staining was observed in the middle of summer (Wood 2002), during hot temperatures, stagnant wind conditions, and low water levels in the reservoir. However, the probe collected data at the end of summer and the beginning of fall, when the atmospheric and water temperatures are beginning to drop and there was more wind. This is significant because, based on Henry's law (Sawyer *et al* 2003) as the water temperature drops the water has a greater capacity for dissolved oxygen and the biological processes that use the available oxygen in the reservoir begin to slow. Henry's law, given in equation 5-1, states that the amount of gas that will dissolve into a liquid, at constant temperature, is proportional to the partial pressure of the gas above the liquid (Sawyer *et al* 2003).

$$K_{H} = \frac{P_{gas}}{C_{equ}}$$
(5.1)

 $P_{gas}$  is the partial pressure of the gas above the water,  $C_{equ}$  is the equilibrium concentration of the gas dissolved into the liquid, and  $K_H$  is the Henry's law constant at a given temperature (Sawyer *et al* 2003).  $K_H$  for water at 20° Celsius is 0.73 atm-m<sup>3</sup>/mol and the atmospheric partial pressure of oxygen at 5000 feet of elevation is 0.16 atm (Sawyer *et al* 2003). Using equation 5.1, the equilibrium DO concentration for Mantua Reservoir is 0.22 mol/m<sup>3</sup> or 7.19 mg/L. Assuming complete mixing with the atmospheric oxygen, Mantua Reservoir would have the above calculated DO concentration.  $K_H$  is sensitive to temperature however, and slight changes in temperatures significantly affect the solubility limits for oxygen.

Spikes in the recorded DO concentration above the theoretical saturation limit of the reservoir could indicate the possibility that an air bubble was resting on the optical sensor of the probe, inflating the recorded DO concentration or that photosynthesis of the aquatic life caused the DO levels to become supersaturated. The sharp drops in DO concentration indicate that there is a lack of mixing in the lower layers of the reservoir with the saturated upper layers and that biological processes are quickly using the available oxygen.

Though the field measurements did not record the hypolimnion in an anaerobic state, the dips indicate that there are regular periods of reduced mixing between the water layers of the reservoir and under the correct conditions could result in anaerobic water in the hypolimnion. Measurements in warmer weather, with warmer water which would reduce the DO capacity of the water, and increased biological activity that would more quickly use the available oxygen would make anaerobic conditions more likely. Deploying the sonde at a greater depth would measure conditions near the sediment-

water interface where there is less mixing of the hypolimnion with the upper reservoir water levels and further increase the likelihood of anaerobic conditions occurring which are favorable for the reduction of ferric iron. Despite the limitations of the field measurements, the regular large drops in DO concentration provide evidence of the ability of Mantua Reservoir to become anaerobic in the lower water levels. This corresponds to the research conducted by Loveless *et al* (1997) which found that the DO levels dropped below acceptable levels in the summer months.

### 5.2 Qualitative Staining Results

I performed qualitative experiments to recreate the staining observed in the Brigham City cemetery and to determine the amount of time necessary for visual staining. This experiment consisted of spraying water saturated with iron onto concrete as described in Section 3.2.

The primary results from this experiment are qualitative observations of the staining evident over a measured period of time. Table 5-1 is the recorded observations at each respective time.

Time	Observations
11:02	Concrete sprayed
12:05	Concrete still drying, no visual
1:03	Iron precipitates visually
2:00	More precipitates on lid
3:00	Faint staining evident on
10:00	Noticeable staining on

Table 5-1: Staining Observations

Figures 5-2 and 5-3 are photographs of the concrete before spraying with water and after the staining occurred and are indicative of the results obtained from the staining experiment. The faint brownish hue, visible in Figure 5-3, is the result of the precipitation of the insoluble ferric iron from the water after being re-aerated by contact with the atmosphere and spraying on the concrete. Though not as visible on the concrete cores, a white surface (a bucket lid), placed under the core to catch the excess water spray, and clearly showed precipitated iron after this experiment. These ferric iron precipitates appeared and caused visible staining approximately two hours after the concrete core was sprayed with anaerobic Mantua Reservoir water. The iron precipitated out of the water before evaporation could take effect to eliminate the water.



**Figure 5-2: Concrete before spraying** 



Figure 5-3: Stained concrete

One difference between the observed field conditions and the qualitative lab experiment is the duration of the exposure. In Brigham City's cemetery, the headstones are exposed to the Mantua water through the irrigation system. A typical zone in an irrigation system is run for approximately 30 minutes. During that time the headstones will be sprayed every few seconds by one or more nearby sprinklers. In contrast, due to the very limited supply of anaerobic Mantua water, I was only able to spray the concrete core continuously for about two minutes. The effect of this difference is that the headstones have the potential for many times the iron exposure and therefore more evident staining. However, as shown by Wallace (2006) staining will only occur when the irrigation water is anaerobic and iron-rich, a condition which will only occur rarely, when the correct conditions happen at Mantua Reservoir.

The difference between the materials sprayed could also change the kinetics of the iron precipitation. The materials in concrete contain high carbonate quantities, giving concrete a basic pH (Mindness *et al* 2003). As seen in the equations that describe the iron oxidation kinetics (equations 2-2, 2-3, 2-5, and 4-1), the rate at which ferrous iron is oxidized to ferric iron is a function of the pH of the system. As the water becomes more basic through contact with the concrete the pH rises and the rate of oxidation is increased. Though the concrete has the potential to increase the oxidation rate of the ferrous iron, the water observed on the bucket lid exhibited precipitated iron quicker than the concrete despite having less contact time as it ran off the concrete. This experiment indicates that staining could occur very rapidly, on the order of a few hours, after spraying the headstones with water.

## 5.3 Quantitative Experimental Results

The purpose of the laboratory experiments was to determine the kinetics of iron oxidation in Mantua Reservoir and provide information that could be used to predict and understand the precipitation reactions. The primary objective was to determine the rate constant (k) that governs the oxidation rate in the reservoir water. This rate constant can then be used in models of the reservoir in order to predict the speed of the reaction and assist in the development of remediation options.

Table 5-2 presents the results of these experiments (described in Section 3.4).Table 5-2 contains the amount of iron in the water from Mantua Reservoir after various

time increments. This table includes the date and time that all of the samples were removed from the bucket of water and also the times that they were actually run in the spectrophotometer. The delay was caused by excessive fouling of the bottle top filters from the suspended sediments. The amount of time between each sample is also included. Table 5-2 also includes the average absorbance measured for each sample and the associated concentration as determined using the calibration curve.

			_				Average
		Time	Run	$\Delta \mathbf{T}$			[Fe]
Date	Sample	Removed	Time	(min)	abs	[Fe] mg/L	mg/L
Oct. 21	1-1	11:25	11:28	0	2.365	9.92	9.87
	1-2				2.344	9.82	
	2-3				NA	NA	8.69
	2-4	11:45	11:55	27	2.083	8.69	
	3-5	12:10	12:20	62	1.706	7.05	7.04
	3-6		12:23	65	1.705	7.04	
	4-7	12:37	12:55	97	1.369	5.58	5.53
	4-8		1:00	102	1.346	5.48	
	5-9	1:35	1:47	149	1.333	5.42	5.43
	5-10		1:50	152	1.339	5.45	
	6-11	3:43	3:55	277	1.662	6.85	6.79
	6-12		3:58	280	1.635	6.74	
	7-13	6:50	7:05	467	0.722	2.76	2.76
	7-14		7:10	472	0.721	2.76	
	8-15	9:10	9:20	542	0.628	2.35	2.33
	8-16		9:23	545	0.619	2.31	
Oct. 22	9-17	3:31	3:48	1650	0.106	0.08	0.07
	9-18		3:51	1653	0.104	0.07	

**Table 5-2: Spectrophotometer Results** 

From these results it is evident that the oxidation and precipitation of ferrous iron in Mantua Reservoir water proceeds quickly. An initial concentration of almost 9.0 mg/L drops to almost nothing in a little over a day. After just two hours, the concentration dropped by about 3.0 mg/L (from 8.69 mg/L to 5.42 mg/L). The first three samples were discarded because I added a couple drops of hydrochloric acid (HCl) to each vial in an effort to acid digest all of the iron. Acid digestion insures that all of the iron that was in solution after filtration remained in solution and did not precipitate (Sawyer *et al* 2003). However, use of the FerroVer reagent eliminates the need for acid digestion. This was realized when the second batch of water was removed and split into two samples (2-3 and 2-4). I added the HCl to sample 2-3 and only added the reagent to 2-4. The samples with the acid turned a milky white color and precipitates settled to the bottom of the vial; the reagent reacted with the HCl in a way which made the sample unusable. Sample 2-4 and all of the subsequent samples produced the expected colorimetric change. Figure 5-4 is a graph of the total time elapsed versus the iron concentration remaining in the water.



Figure 5-4: Iron oxidation over time

Figure 5-4 includes a trend line, its associated exponential equation, and an R-squared value. R-squared for this trend line is 0.9779. Removing the outlier point and using the average time elapsed and concentration yields Figure 5-5.



Figure 5-5: Revised iron oxidation over time

By removing the outlier point the R-squared value moves closer to one, with a value of 0.9918, indicating that the trend line is a better fit to the data. Equation 5-2 is the equation for the revised trend line:

$$y = 8.9877e^{-0.0029x} \tag{5-2}$$

where x is the time in minutes and y is the iron concentration in mg/L remaining in the water. This equation is the form of equation 2-4 describing first-order kinetics with x corresponding to t and y to C. This gives a rate constant k for Mantua Reservoir water of 0.0029 min<sup>-1</sup>, based on my experimental results

# 5.4 PHREEQC Model Results

Mantua Reservoir was first modeled using the default rate constant provided with the iron oxidation kinetics example (see equation 4-1 and Section 4.2). The model-produced result is a plot of the change in concentration of both ferrous iron ( $Fe^{2+}$ ) and ferric iron ( $Fe^{3+}$ ) versus time. Figure 5-6 is the plot produced using the default rate constant.



Figure 5-6: Change in iron concentration using default k

As the ferric iron concentration rises, due to the solubility product being extremely low ( $K_{sp}$ = 2.79x10<sup>-39</sup>), the aqueous solution becomes supersaturated with respect to iron (III) (Sawyer *et al* 2003). The insoluble ferric iron will then begin to precipitate out of the solution. Using the default rate constant, after five days the ferrous iron concentration in the water has dropped by fifty percent. However, this model does not cause the oxidation to occur at close to the same rate as seen experimentally, with the experimental and observed reaction rates being much faster. Again, this discrepancy is probably the result of a biological component to the iron oxidation as was discussed in Section 2.3.

In order to more accurately predict the iron oxidation kinetics in Mantua Reservoir water, the model was modified to use the measured kinetic data from my laboratory experiments. Through a trial and error process of adjusting the rate constant, I created a model that closely matched the experimental data. Figure 5-7 is a plot of the concentration of ferrous iron over time based on the revised model and on the experimental data.

The rate constant found was  $4 \times 10^{13}$ /atm x min, thirty times bigger than the default value. This value is different than the one shown in Figure 5-5 because a different kinetics equation was used in the PHREEQC model rather than the first-order model presented above. Using the fitted theoretical rate constant from calibrating the PHREEQC model to the laboratory results, the complete oxidation of ferrous iron in Mantua Reservoir water was modeled.

Figure 5-8 presents the same parameters as Figure 5-6, but the data were calculated by applying the calibrated rate constant from the Mantua water experimental



Figure 5-7: Model vs experimental iron concentrations



Figure 5-8: Model of Mantua iron oxidation kinetics

results. Figure 5-8 shows that after one day there is virtually no ferrous iron (0.15 mg/L) remaining in the reservoir water and after only four hours half of the ferrous iron dissolved in the water has been oxidized to ferric iron. This matches both observations and laboratory experiments. This also matches the staining events in the Brigham City cemetery, where staining occurred overnight and no stain build-up was noticed.

I propose that the explanation for the difference in the rate constants between the PHREEQC example model and the Mantua water model is the catalytic effects of microorganisms. As Okereke and Stevens (1991) proved with their research, the presence of iron oxidizing bacteria greatly increases the rate of iron oxidation. The presence of microbes can accelerate the reaction rate by a factor of 10<sup>6</sup> (Singer and Stumm 1970). *Thiobacillus ferrooxidans* are the most common microbes that oxidize ferric iron. Based on the research of Okereke and Stevens (1991), the right microbes could easily accelerate the kinetics of iron oxidation by an order of magnitude which would account for the differences found.

# 6 Conclusions

The purpose of this research was to confirm the capacity of Mantua Reservoir to achieve anaerobic conditions, causing the reduction and eventual oxidation of iron, and to determine the ferrous iron oxidation kinetics and thus how quickly staining could occur. Knowing the rate of the oxidation reaction will assist in the determination of practical remediation efforts by determining the residence time of the water after treatment before it could be used in the irrigation system.

The efforts to confirm the potential for Mantua Reservoir revealed that even in early fall, the DO concentration in the hypolimnion fluctuates severely. Though the study was conducted when the water temperature was already decreasing, causing an increase in the potential equilibrium DO concentration, the fact that the DO levels oscillated gave evidence that anaerobic conditions are likely in the lower water layers of Mantua Reservoir during the warmer summer conditions. The field data collected confirmed the results obtained by Loveless *et al* (1997) as part of the Clean Lakes Study. Their field work found DO levels as low as 3.0 mg/L within a meter of the bottom. Anaerobic conditions are required for the reduction of ferric iron, which is found in abundance in Mantua sediments. Reduced iron, in the ferrous state, is much more soluble than ferric iron and dissolves into the water only to be oxidized upon re-aeration through the irrigation system (Sawyer *et al* 2003). The iron oxidation kinetics for Mantua Reservoir were determined using three different methods. The first method was a qualitative observation of the staining caused by iron precipitation on a cement core. Though the conditions of the experimentally derived staining differed from the field conditions, iron precipitation was evident after only two hours of observation. This showed that if the anaerobic conditions existed in Mantua Reservoir resulting in high amounts of dissolved iron, the use of the pressurized irrigation system would cause staining to appear on the headstones within a matter of hours.

The experimental results of the iron oxidation for Mantua yielded results that showed the iron was quickly oxidized and precipitated from the Mantua water. The ferrous iron was almost completely gone after 26 hours and had been reduced by over a third in just a couple of hours. Fitting a simple first order kinetics equation to the experimental data yielded a rate constant of 0.0029 min<sup>-1</sup>, giving a half life of 239 minutes or approximately 4 hours. As with the qualitative results, the kinetics experiment has proved that the iron will precipitate out of the water and cause staining in Brigham City.

The creation of a geochemical computer model, using PHREEQC, also confirmed the speed of the iron oxidation kinetics. Using an example provided with the software as a foundation, and modifying the example to match the measured physical and chemical properties of Mantua Reservoir, resulted in a model in which the computed ferrous iron concentration dropped by fifty percent over the course of five days. This was not a good fit to the experimental data and therefore the model was calibrated to the experimental results from the actual Mantua water. The rate constant in the calibrated model was

 $4x10^{13}$ /atm x min. With the rate constant calibrated to experimental results and a computer model of the oxidation kinetics, the oxidation of iron was predicted for any changing conditions of the reservoir. Model calculations showed that the majority of the iron would precipitate in a few hours.

### 6.1 Application

Knowing the iron oxidation kinetics of Mantua Reservoir water makes remediation recommendations possible. The purpose of this section is not to exhaustively study all of the technology available for the removal of dissolved iron in water but rather to provide an overview of possibilities for Brigham City to employ at Mantua Reservoir or in their irrigation system. (For a comprehensive study on iron treatments refer to *Iron and Manganese Treatment for Small Systems*, a thesis prepared by Harry Campbell for Brigham Young University, 1989).

There are two general approaches that could be applied. The first and recommended approach is to change conditions at Mantua Reservoir so that the hypolimnion does not become anaerobic. In addition to addressing the staining problem, this approach has the potential to address several other problems noted at Mantua including water quality and aesthetics. The second approach is to treat iron rich water after it leaves Mantua Reservoir before being used for irrigation.

The simplest and preferred solution to the staining problem would be to prevent iron from dissolving from the sediment under anaerobic conditions. Prevention would involve precluding the reservoir from becoming anaerobic in the hypolimnion by aeration or circulation. There are numerous commercial systems designed to aerate lagoons and

reservoirs that could potentially be used at Mantua. During the course of my lab experiments, there were numerous failed attempts to conduct the experimental phase of the kinetics investigation. Invariably the failure was a consequence of excessive DO in the water preventing iron from dissolving from the sediments, as little as 2.0 mg/L, in the water sample. (The one successful attempt had a DO concentration of 1.0 mg/L after opening the bucket and mixing to a small degree by using a field DO probe which might have caused some of the DO in solution). In any cases where the water contained measurable amounts of DO, after testing with the spectrophotometer, these failed tests only included trace amounts of iron because the iron was never dissolved from the sediments.

From these failures, I learned that very little oxygen is necessary to prevent the dissolution of iron from the sediments. As a result, remediation methods that increase the dissolved oxygen in the hypolimnion would successfully prevent ferric iron from being reduced and then dissolved as ferrous iron into the water column. Diffusers laid on the bed of the reservoir, near the outlet, would prevent the system from going anaerobic and also oxidize any iron already dissolved in the water causing it to precipitate and settle out before reaching the irrigation system. Another preventative measure would be to put a floating mixer anchored in the area of the outlet (this area is already restricted to recreational activities). This would have the effect of mixing the DO saturated surface waters with lower layers that have the greatest potential for becoming anaerobic. Like the diffusers this would prevent the microorganisms from using the ferric iron found in the reservoir sediments as an electron acceptor and would oxidize any ferrous iron

dissolved in the water. Both types of systems, and others such as sprayers and mixers, are commercially available.

The second general category is treating the water before irrigation. The basic idea of iron removal most commonly employed is the oxidation of the ferrous iron and subsequent clarification of the water, either using filtration or precipitation (Campbell 1989). This is exactly the process that is occurring in the system comprising Mantua Reservoir and the Brigham City secondary irrigation system. The major difference is the location of the removal of the iron hydroxide precipitates. In an engineered process they will be either removed in a settling basin or using a filtration system (Campbell 1989). In Brigham City's system the iron precipitates settle out on the headstones of the cemetery.

A solution would be to cause the iron to settle out, after oxidation, in a controlled location. This could be as simple as cascading the water over rocks, or other obstacles, far enough up the system to allow the iron (III) a chance to settle out. Immediately below the dam, before entering the penstock would allow treatment while retaining the pressure head required for power generation. The cascading water would be re-aerated and cause the oxidation of the ferrous iron. The reaction rate is fast enough, as determined by this study, to cause the iron to oxidize and settle out before entering the penstock and reaching the sprinklers of the city irrigation system. To prevent the iron precipitates from causing problems in the pipe distribution network a small settling pond, with a hydraulic detention time of a couple of hours, could be placed after the cascade to give the majority of the iron hydroxides a place to settle out.
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# Appendix A. Field Data

### Table A-1: Field Data Collected from Mantua Reservoir (24 hour period, 9/11/2006)

MDV         C         (mgL)         KOmm.cm         git         ppt         mS/cm         %           9/11/2006 0:15         19.38         6.07         584         0.125         0.09         0.192         87.7           9/11/2006 0:45         19.33         7.93         5.84         0.125         0.09         0.192         88.4           9/11/2006 0:45         19.37         7.86         5.84         0.125         0.09         0.192         88.4           9/11/2006 1:15         19.37         7.81         5.84         0.125         0.09         0.192         88.4           9/11/2006 1:45         19.31         7.8         5.85         0.125         0.09         0.192         84.6           9/11/2006 1:45         19.23         7.75         5.85         0.125         0.09         0.192         84.6           9/11/2006 2:45         19.22         7.3         5.85         0.125         0.09         0.192         80.3           9/11/2006 3:00         19.21         7.33         5.86         0.125         0.09         0.192         79.1           9/11/2006 3:30         19.14         6.98         5.86         0.125         0.09         0.192         77.2	DateTime	Temp	ODO Conc	Resistivity	TDS	Salinity	SpCond	000%
9r11/2006 0.00         19.39         7.97         5.83         0.125         0.19         86.7           9r11/2006 0.30         19.38         7.93         5.84         0.125         0.09         0.192         87.7           9r11/2006 0.30         19.38         7.93         5.84         0.125         0.09         0.192         86.2           9r11/2006 1.30         19.37         7.81         5.84         0.125         0.09         0.192         86.4           9r11/2006 1.30         19.33         7.85         5.84         0.125         0.09         0.192         86.1           9r11/2006 1.45         19.33         7.85         5.84         0.125         0.09         0.192         84.6           9r11/2006 1.45         19.33         7.85         5.85         0.125         0.09         0.192         84.6           9r11/2006 2.30         19.24         7.41         5.85         0.125         0.09         0.192         78.4           9r11/2006 3.30         19.14         6.98         5.86         0.125         0.09         0.192         79.4           9r11/2006 3.30         19.14         6.98         5.86         0.125         0.09         0.192         74.5 <td>M/D/Y</td> <td>C</td> <td>(ma/L)</td> <td>KOhm.cm</td> <td>a/L</td> <td>ppt</td> <td>mS/cm</td> <td>%</td>	M/D/Y	C	(ma/L)	KOhm.cm	a/L	ppt	mS/cm	%
9/11/2006 0:15         19.38         7.07         5.84         0.125         0.09         0.192         87.7           9/11/2006 0:00         19.37         7.86         5.84         0.125         0.09         0.192         86.4           9/11/2006 1:15         19.37         7.81         5.84         0.125         0.09         0.192         86.1           9/11/2006 1:15         19.37         7.83         5.84         0.125         0.09         0.192         86.2           9/11/2006 1:45         19.31         7.8         5.85         0.125         0.09         0.192         84.6           9/11/2006 2:15         19.27         7.75         5.85         0.125         0.09         0.192         84.3           9/11/2006 2:16         19.24         7.41         5.85         0.125         0.09         0.192         79.4           9/11/2006 3:00         19.21         7.3         5.86         0.125         0.09         0.192         79.4           9/11/2006 3:45         19.14         6.98         5.86         0.125         0.09         0.192         74.9           9/11/2006 4:45         19.14         6.91         5.86         0.125         0.09         0.192 <td>9/11/2006 0:00</td> <td>19.39</td> <td>7.97</td> <td>5.83</td> <td>0.125</td> <td>0.09</td> <td>0.192</td> <td>86.7</td>	9/11/2006 0:00	19.39	7.97	5.83	0.125	0.09	0.192	86.7
9/11/2006 0.30         19.38         7.93         5.84         0.125         0.09         0.192         88.2           9/11/2006 1.00         19.37         7.81         5.84         0.125         0.09         0.192         86.4           9/11/2006 1.15         19.37         7.81         5.84         0.125         0.09         0.192         86.1           9/11/2006 1.45         19.33         7.85         5.84         0.125         0.09         0.192         84.6           9/11/2006 2.00         19.29         7.75         5.85         0.125         0.09         0.192         84.6           9/11/2006 2.01         19.24         7.41         5.85         0.125         0.09         0.192         81.5           9/11/2006 2.01         19.24         7.41         5.85         0.125         0.09         0.192         79.1           9/11/2006 3.00         19.21         7.33         5.86         0.125         0.09         0.192         77.2           9/11/2006 3.05         19.14         6.92         5.86         0.125         0.09         0.192         76.1           9/11/2006 4.05         19.14         6.92         5.86         0.125         0.09         0.192 </td <td>9/11/2006 0:15</td> <td>19.38</td> <td>8.07</td> <td>5.84</td> <td>0.125</td> <td>0.09</td> <td>0.192</td> <td>87.7</td>	9/11/2006 0:15	19.38	8.07	5.84	0.125	0.09	0.192	87.7
9/11/2006 0.45         19.37         7.86         5.84         0.125         0.09         0.192         85.4           9/11/2006 1:15         19.37         7.81         5.84         0.125         0.09         0.192         85.2           9/11/2006 1:45         19.33         7.85         5.84         0.125         0.09         0.192         85.2           9/11/2006 1:45         19.31         7.8         5.85         0.125         0.09         0.192         84.6           9/11/2006 1:45         19.31         7.8         5.85         0.125         0.09         0.192         84.3           9/11/2006 2:15         19.24         7.41         5.85         0.125         0.09         0.192         79.4           9/11/2006 3:00         19.21         7.33         5.85         0.125         0.09         0.192         77.2           9/11/2006 3:03         19.14         6.98         5.86         0.125         0.09         0.192         74.9           9/11/2006 3:30         19.14         6.92         5.86         0.125         0.09         0.192         74.7           9/11/2006 4:15         19.07         6.81         5.86         0.125         0.09         0.192 <td>9/11/2006 0:30</td> <td>19.38</td> <td>7.93</td> <td>5.84</td> <td>0.125</td> <td>0.09</td> <td>0.192</td> <td>86.2</td>	9/11/2006 0:30	19.38	7.93	5.84	0.125	0.09	0.192	86.2
9/11/2006         10.10         10.37         7.81         5.84         0.125         0.09         0.192         84.9           9/11/2006         1.15         19.37         7.85         5.84         0.125         0.09         0.192         86.1           9/11/2006         1.45         19.31         7.85         5.85         0.125         0.09         0.192         84.6           9/11/2006         2.01         19.27         7.55         5.85         0.125         0.09         0.192         81.5           9/11/2006         2.30         19.24         7.41         5.85         0.125         0.09         0.192         79.1           9/11/2006         2.30         19.24         7.41         5.85         0.125         0.09         0.192         79.1           9/11/2006         3.01         9.14         6.92         5.86         0.125         0.09         0.192         75.5           9/11/2006         3.19         1.4         6.92         5.86         0.125         0.09         0.192         76.1           9/11/2006         3.45         19.14         6.92         5.86         0.125         0.09         0.192         76.1	9/11/2006 0:45	19.37	7.86	5.84	0.125	0.09	0.192	85.4
9/11/2006 1:16         19.37         7.83         5.84         0.125         0.09         0.192         86.1           9/11/2006 1:45         19.31         7.8         5.85         0.125         0.09         0.192         84.6           9/11/2006 2:00         19.29         7.75         5.85         0.125         0.09         0.192         84.6           9/11/2006 2:15         19.24         7.41         5.85         0.125         0.09         0.192         81.5           9/11/2006 2:45         19.24         7.41         5.85         0.125         0.09         0.192         77.1           9/11/2006 3:30         19.14         6.86         5.86         0.125         0.09         0.192         77.2           9/11/2006 3:30         19.14         6.92         5.86         0.125         0.09         0.192         76.1           9/11/2006 4:00         19.14         6.92         5.86         0.125         0.09         0.192         76.2           9/11/2006 4:01         19.14         6.92         5.86         0.125         0.09         0.192         76.2           9/11/2006 6:15         19.07         6.81         5.86         0.125         0.09         0.192 <td>9/11/2006 1:00</td> <td>19.37</td> <td>7.81</td> <td>5.84</td> <td>0.125</td> <td>0.09</td> <td>0.192</td> <td>84.9</td>	9/11/2006 1:00	19.37	7.81	5.84	0.125	0.09	0.192	84.9
9/11/2006         1:30         1         7.85         5.84         0.125         0.09         0.192         85.2           9/11/2006         1:0         19.29         7.75         5.85         0.125         0.09         0.192         84.6           9/11/2006         2:00         19.29         7.75         5.85         0.125         0.09         0.192         84.3           9/11/2006         2:30         19.24         7.41         5.85         0.125         0.09         0.192         78.1           9/11/2006         3:00         19.21         7.33         5.86         0.125         0.09         0.192         77.2           9/11/2006         3:01         19.14         6.92         5.86         0.125         0.09         0.192         74.7           9/11/2006         3:45         19.14         7.03         5.86         0.125         0.09         0.192         76.1           9/11/2006         4:15         19.07         6.81         5.86         0.125         0.09         0.192         71.8           9/11/2006         19.02         6.86         5.86         0.125         0.09         0.192         71.8           9/11/2006 <t< td=""><td>9/11/2006 1:15</td><td>19.37</td><td>7.93</td><td>5.84</td><td>0.125</td><td>0.09</td><td>0.192</td><td>86.1</td></t<>	9/11/2006 1:15	19.37	7.93	5.84	0.125	0.09	0.192	86.1
9/11/2006         1:46         19:25         7.75         5.85         0.125         0.09         0.192         84           9/11/2006         19:25         7.52         5.85         0.125         0.09         0.192         81.5           9/11/2006         2:30         19:24         7.41         5.85         0.125         0.09         0.192         79.1           9/11/2006         2:45         19:22         7.3         5.86         0.125         0.09         0.192         77.2           9/11/2006         3:0         19:14         6.98         5.86         0.125         0.09         0.192         77.5           9/11/2006         3:0         19:14         6.92         5.86         0.125         0.09         0.192         76.1           9/11/2006         4:10         19:14         6.92         5.86         0.125         0.09         0.192         76.1           9/11/2006         4:10         19:14         6.91         5.86         0.125         0.09         0.192         77.5           9/11/2006         5:15         19:07         6.81         5.86         0.125         0.09         0.192         71.4           9/11/2006 <t< td=""><td>9/11/2006 1:30</td><td>19.33</td><td>7.85</td><td>5.84</td><td>0.125</td><td>0.09</td><td>0.192</td><td>85.2</td></t<>	9/11/2006 1:30	19.33	7.85	5.84	0.125	0.09	0.192	85.2
9/11/2006 2:00         19.29         7.75         5.85         0.125         0.09         0.192         84           9/11/2006 2:30         19.24         7.41         5.85         0.125         0.09         0.192         80.3           9/11/2006 2:30         19.24         7.41         5.85         0.125         0.09         0.192         79.4           9/11/2006 3:00         19.21         7.33         5.85         0.125         0.09         0.192         77.4           9/11/2006 3:01         19.14         6.98         5.86         0.125         0.09         0.192         77.4           9/11/2006 3:45         19.14         6.92         5.86         0.125         0.09         0.192         74.7           9/11/2006 4:15         19.14         7.03         5.86         0.125         0.09         0.192         74.7           9/11/2006 4:15         19.12         6.66         5.86         0.125         0.09         0.192         74.7           9/11/2006 4:45         19.07         6.68         5.86         0.125         0.09         0.192         71.2           9/11/2006 6:30         19.02         6.68         5.86         0.125         0.9         0.192	9/11/2006 1:45	19.31	7.8	5.85	0.125	0.09	0.192	84.6
9/11/2006 2:15         19.25         7.52         5.85         0.125         0.09         0.192         81.5           9/11/2006 2:45         19.22         7.3         5.85         0.125         0.09         0.192         79.1           9/11/2006 2:45         19.21         7.33         5.85         0.125         0.09         0.192         77.2           9/11/2006 3:15         19.19         7.13         5.86         0.125         0.09         0.192         77.2           9/11/2006 3:45         19.14         6.92         5.86         0.125         0.09         0.192         76.1           9/11/2006 4:00         19.14         7.03         5.86         0.125         0.09         0.192         76.1           9/11/2006 4:30         19.12         6.66         5.87         0.125         0.09         0.192         73.5           9/11/2006 5:15         19.01         6.66         5.87         0.125         0.09         0.192         73.8           9/11/2006 5:45         19         6.77         5.87         0.125         0.09         0.193         73.3           9/11/2006 6:45         19.02         6.68         5.86         0.125         0.09         0.192	9/11/2006 2:00	19.29	7.75	5.85	0.125	0.09	0.192	84
9111/2006 2:30         19.24         7.41         5.85         0.125         0.09         0.192         80.3           9111/2006 2:45         19.22         7.3         5.85         0.125         0.09         0.192         79.4           9111/2006 3:00         19.21         7.33         5.86         0.125         0.09         0.192         77.4           9111/2006 3:30         19.14         6.98         5.86         0.125         0.09         0.192         74.9           9111/2006 4:45         19.14         6.92         5.86         0.125         0.09         0.192         74.7           9111/2006 4:15         19.14         6.91         5.86         0.125         0.09         0.192         74.7           9111/2006 4:30         19.12         6.96         5.86         0.125         0.09         0.192         75.5           9111/2006 6:15         19.01         6.6         5.86         0.125         0.09         0.192         74.7           9111/2006 6:15         19.02         6.68         5.86         0.125         0.09         0.192         72.1           9111/2006 6:15         18.97         6.72         5.88         0.125         0.09         0.192 <td>9/11/2006 2:15</td> <td>19.25</td> <td>7.52</td> <td>5.85</td> <td>0.125</td> <td>0.09</td> <td>0.192</td> <td>81.5</td>	9/11/2006 2:15	19.25	7.52	5.85	0.125	0.09	0.192	81.5
9/11/2006 2:45         19.21         7.3         5.85         0.125         0.09         0.192         79.4           9/11/2006 3:15         19.9         7.13         5.86         0.125         0.09         0.192         77.2           9/11/2006 3:30         19.14         6.98         5.86         0.125         0.09         0.192         74.9           9/11/2006 3:45         19.14         6.92         5.86         0.125         0.09         0.192         74.7           9/11/2006 4:00         19.14         7.03         5.86         0.125         0.09         0.192         74.7           9/11/2006 4:30         19.12         6.96         5.86         0.125         0.09         0.192         75.5           9/11/2006 6:00         19.02         6.66         5.87         0.125         0.09         0.192         73.5           9/11/2006 6:30         19.02         6.68         5.86         0.125         0.09         0.193         73           9/11/2006 6:43         19.01         6.6         5.88         0.125         0.09         0.192         72.1           9/11/2006 6:45         19.02         6.68         5.86         0.125         0.09         0.192	9/11/2006 2:30	19.24	7.41	5.85	0.125	0.09	0.192	80.3
9/11/2006 3:00         19.21         7.33         5.85         0.125         0.09         0.192         79.4           9/11/2006 3:30         19.14         6.98         5.86         0.125         0.09         0.192         77.2           9/11/2006 3:45         19.14         6.92         5.86         0.125         0.09         0.192         74.9           9/11/2006 4:15         19.14         7.03         5.86         0.125         0.09         0.192         76.1           9/11/2006 4:15         19.11         6.91         5.86         0.125         0.09         0.192         75.2           9/11/2006 4:45         19.07         6.81         5.86         0.125         0.09         0.192         73.5           9/11/2006 5:15         19.01         6.6         5.86         0.125         0.09         0.193         73.3           9/11/2006 5:30         19.02         6.68         5.86         0.125         0.09         0.193         73.5           9/11/2006 6:50         18.97         6.72         5.88         0.125         0.09         0.192         70.7           9/11/2006 6:15         18.92         6.57         5.88         0.125         0.09         0.192 <td>9/11/2006 2:45</td> <td>19.22</td> <td>7.3</td> <td>5.85</td> <td>0.125</td> <td>0.09</td> <td>0.192</td> <td>79.1</td>	9/11/2006 2:45	19.22	7.3	5.85	0.125	0.09	0.192	79.1
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	9/11/2006 3:00	19.21	7.33	5.85	0.125	0.09	0.192	79.4
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	9/11/2006 3:15	19.19	7.13	5.86	0.125	0.09	0.192	77.2
9/11/2006         9.14         6.92         5.86         0.125         0.09         0.192         74.9           9/11/2006         4:00         19.14         7.03         5.86         0.125         0.09         0.192         76.1           9/11/2006         4:15         19.11         6.91         5.86         0.125         0.09         0.192         75.2           9/11/2006         5:00         19.02         6.66         5.87         0.125         0.09         0.192         71.8           9/11/2006         5:10         19.01         6.6         5.86         0.125         0.09         0.193         71.2           9/11/2006         5:30         19.02         6.68         5.86         0.125         0.09         0.193         73.3           9/11/2006         6:45         19         6.77         5.88         0.125         0.09         0.192         70.7           9/11/2006         18.97         6.77         5.88         0.125         0.09         0.192         72.1           9/11/2006         18.91         6.64         5.89         0.125         0.09         0.192         72.9           9/11/2006         18.93         6.77         <	9/11/2006 3:30	19.14	6.98	5.86	0.125	0.09	0.192	75.5
9/11/2006 4:00         19.14         7.03         5.86         0.125         0.09         0.192         76.1           9/11/2006 4:15         19.11         6.91         5.86         0.125         0.09         0.192         74.7           9/11/2006 4:45         19.07         6.81         5.86         0.125         0.09         0.192         73.5           9/11/2006 5:15         19.02         6.66         5.87         0.125         0.09         0.192         71.8           9/11/2006 5:15         19.02         6.68         5.86         0.125         0.09         0.193         71.2           9/11/2006 5:30         19.02         6.68         5.86         0.125         0.09         0.193         72.1           9/11/2006 6:00         18.97         6.77         5.87         0.125         0.09         0.192         72.5           9/11/2006 6:30         18.91         6.64         5.89         0.125         0.09         0.192         72.1           9/11/2006 6:45         18.93         6.77         5.88         0.125         0.09         0.192         72.1           9/11/2006 7:00         18.93         6.77         5.88         0.125         0.09         0.192 </td <td>9/11/2006 3:45</td> <td>19.14</td> <td>6.92</td> <td>5.86</td> <td>0.125</td> <td>0.09</td> <td>0.192</td> <td>74.9</td>	9/11/2006 3:45	19.14	6.92	5.86	0.125	0.09	0.192	74.9
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	9/11/2006 4:00	19.14	7.03	5.86	0.125	0.09	0.192	76.1
9/11/2006 4:30         19.12         6.96         5.86         0.125         0.09         0.192         75.2           9/11/2006 4:35         19.07         6.81         5.86         0.125         0.09         0.192         73.5           9/11/2006 5:10         19.02         6.66         5.87         0.125         0.09         0.193         71.2           9/11/2006 5:15         19.01         6.6         5.86         0.125         0.09         0.193         73.3           9/11/2006 5:45         19         6.77         5.87         0.125         0.09         0.192         72.5           9/11/2006 6:30         18.91         6.64         5.89         0.125         0.09         0.192         72.5           9/11/2006 6:30         18.91         6.64         5.89         0.125         0.09         0.192         71.4           9/11/2006 6:45         18.93         6.77         5.88         0.125         0.09         0.192         72.9           9/11/2006 7:15         18.88         6.68         5.89         0.125         0.09         0.192         72.2           9/11/2006 7:30         18.91         6.71         5.89         0.125         0.09         0.192	9/11/2006 4.15	19 11	6.91	5.86	0 125	0.09	0 192	74 7
9/11/2006 4:45       19.07       6.81       5.86       0.125       0.09       0.192       73.5         9/11/2006 5:00       19.02       6.66       5.87       0.125       0.09       0.193       71.2         9/11/2006 5:30       19.02       6.68       5.86       0.125       0.09       0.193       72.1         9/11/2006 5:30       19.02       6.68       5.86       0.125       0.09       0.193       73.5         9/11/2006 5:45       19       6.77       5.87       0.125       0.09       0.192       72.5         9/11/2006 6:30       18.97       6.72       5.88       0.125       0.09       0.192       71.4         9/11/2006 6:30       18.91       6.64       5.89       0.125       0.09       0.192       72.1         9/11/2006 7:00       18.93       6.7       5.88       0.125       0.09       0.192       72.9         9/11/2006 7:45       18.88       6.68       5.89       0.125       0.09       0.192       72.9         9/11/2006 7:45       18.86       6.68       5.89       0.125       0.09       0.192       72.6         9/11/2006 7:45       18.86       6.75       5.9       0.125 <td>9/11/2006 4:30</td> <td>19.12</td> <td>6.96</td> <td>5.86</td> <td>0.125</td> <td>0.09</td> <td>0.192</td> <td>75.2</td>	9/11/2006 4:30	19.12	6.96	5.86	0.125	0.09	0.192	75.2
9/11/2006 5:0019.026.665.870.1250.090.19271.89/11/2006 5:3019.026.685.860.1250.090.19371.29/11/2006 5:3019.026.685.860.1250.090.19372.19/11/2006 6:3018.976.725.880.1250.090.19272.59/11/2006 6:1518.926.575.880.1250.090.19270.79/11/2006 6:3018.916.645.890.1250.090.19271.49/11/2006 6:4518.936.75.880.1250.090.19272.19/11/2006 7:0018.936.775.880.1250.090.19272.99/11/2006 7:3018.96.715.890.1250.090.19272.29/11/2006 7:4518.866.755.90.1250.090.19272.69/11/2006 8:1518.946.755.890.1250.090.19272.79/11/2006 8:3018.856.715.90.1250.090.19272.79/11/2006 8:3018.856.715.90.1250.090.19272.79/11/2006 8:3018.866.955.90.1250.090.19277.79/11/2006 8:3018.866.955.90.1250.090.19277.59/11/2006 8:3018.866.955.90.1250.090.19277.59/11/2006 8:30 <t< td=""><td>9/11/2006 4:45</td><td>19.07</td><td>6.81</td><td>5.86</td><td>0.125</td><td>0.09</td><td>0.192</td><td>73.5</td></t<>	9/11/2006 4:45	19.07	6.81	5.86	0.125	0.09	0.192	73.5
9/11/20065:1519.016.65.860.1250.090.19371.29/11/20065:3019.026.685.860.1250.090.193739/11/20066:0018.976.775.870.1250.090.19272.59/11/20066:1518.926.575.880.1250.090.19270.79/11/20066:3018.916.645.890.1250.090.19271.49/11/20066:4518.936.775.880.1250.090.19272.19/11/20067:0018.936.775.880.1250.090.19272.99/11/20067:3018.96.715.890.1250.090.19272.99/11/20067:3018.96.715.890.1250.090.19272.69/11/20067:3018.916.845.890.1250.090.19272.79/11/20067:4518.866.755.90.1250.090.19272.79/11/20068:3018.856.715.90.1250.090.19272.79/11/20068:3018.866.955.90.1250.090.19274.79/11/20068:4518.846.645.90.1250.090.19277.39/11/20068:1518.947.315.890.1250.090.19277.39/11/20069:10<	9/11/2006 5:00	19.02	6.66	5.87	0.125	0.09	0.192	71.8
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	9/11/2006 5:15	19.01	6.6	5.86	0.125	0.09	0 193	71.2
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	9/11/2006 5:30	19.02	6 68	5.86	0.125	0.09	0 193	72.1
9/11/2006         18.97         6.72         5.88         0.125         0.09         0.192         72.5           9/11/2006         6:15         18.92         6.57         5.88         0.125         0.09         0.192         70.7           9/11/2006         6:43         18.91         6.64         5.89         0.125         0.09         0.192         72.1           9/11/2006         6:45         18.93         6.77         5.88         0.125         0.09         0.192         72.1           9/11/2006         7:00         18.93         6.77         5.88         0.125         0.09         0.192         72.9           9/11/2006         7:15         18.86         6.68         5.89         0.125         0.09         0.192         72.6           9/11/2006         7:45         18.86         6.75         5.9         0.125         0.09         0.192         72.6           9/11/2006         8:01         18.91         6.84         5.89         0.125         0.09         0.192         72.7           9/11/2006         8:30         18.85         6.71         5.9         0.125         0.09         0.192         74.7           9/11/2006	9/11/2006 5:45	19	6 77	5.87	0.125	0.09	0 193	73
9/11/2006 6:15       18.92       6.57       5.88       0.125       0.09       0.192       70.7         9/11/2006 6:30       18.91       6.64       5.89       0.125       0.09       0.192       71.4         9/11/2006 6:45       18.93       6.7       5.88       0.125       0.09       0.192       72.1         9/11/2006 7:00       18.93       6.77       5.88       0.125       0.09       0.192       72.9         9/11/2006 7:15       18.88       6.68       5.89       0.125       0.09       0.192       72.2         9/11/2006 7:30       18.9       6.71       5.89       0.125       0.09       0.192       72.2         9/11/2006 8:00       18.91       6.84       5.89       0.125       0.09       0.192       72.7         9/11/2006 8:15       18.94       6.75       5.89       0.125       0.09       0.192       72.7         9/11/2006 8:30       18.85       6.71       5.9       0.125       0.09       0.192       72.7         9/11/2006 8:45       18.84       6.64       5.9       0.125       0.09       0.192       75.9         9/11/2006 9:50       18.84       7.18       5.9       0.125 <td>9/11/2006 6:00</td> <td>18.97</td> <td>6.72</td> <td>5.88</td> <td>0.125</td> <td>0.09</td> <td>0 192</td> <td>72.5</td>	9/11/2006 6:00	18.97	6.72	5.88	0.125	0.09	0 192	72.5
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	9/11/2006 6:15	18.92	6.57	5.88	0.125	0.09	0.192	70.7
9/11/2006       6:45       18.93       6.7       5.88       0.125       0.09       0.192       72.1         9/11/2006       7:00       18.93       6.77       5.88       0.125       0.09       0.192       72.9         9/11/2006       7:15       18.88       6.68       5.89       0.125       0.09       0.192       72.2         9/11/2006       7:15       18.86       6.675       5.9       0.125       0.09       0.192       72.2         9/11/2006       7:45       18.86       6.75       5.9       0.125       0.09       0.192       72.6         9/11/2006       8:00       18.91       6.84       5.89       0.125       0.09       0.192       72.7         9/11/2006       8:01       18.85       6.71       5.9       0.125       0.09       0.192       72.7         9/11/2006       8:01       18.85       6.71       5.9       0.125       0.09       0.192       72.7         9/11/2006       8:03       18.86       6.95       5.9       0.125       0.09       0.192       74.7         9/11/2006       9:01       18.86       7.89       0.125       0.09       0.192       77.3	9/11/2006 6:30	18.91	6 64	5.89	0.125	0.09	0 192	71.4
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	9/11/2006 6:45	18.93	6.7	5.88	0.125	0.09	0.192	72.1
9/11/2006 7:15       18.88       6.68       5.89       0.125       0.09       0.192       71.9         9/11/2006 7:30       18.9       6.71       5.89       0.125       0.09       0.192       72.2         9/11/2006 7:45       18.86       6.75       5.9       0.125       0.09       0.192       72.2         9/11/2006 8:00       18.91       6.84       5.89       0.125       0.09       0.192       72.2         9/11/2006 8:15       18.94       6.75       5.89       0.125       0.09       0.192       72.2         9/11/2006 8:15       18.84       6.64       5.9       0.125       0.09       0.192       72.2         9/11/2006 8:45       18.84       6.64       5.9       0.125       0.09       0.192       74.7         9/11/2006 9:00       18.86       6.95       5.9       0.125       0.09       0.192       74.7         9/11/2006 9:15       18.91       7.05       5.9       0.125       0.09       0.192       78.7         9/11/2006 9:45       18.94       7.31       5.89       0.125       0.09       0.192       78.7         9/11/2006 10:00       19       7.45       5.89       0.125	9/11/2006 7·00	18.93	6 77	5.88	0.125	0.09	0 192	72.9
9/11/2006 7:30         18.9         6.71         5.89         0.125         0.09         0.192         72.2           9/11/2006 7:45         18.86         6.75         5.9         0.125         0.09         0.192         72.6           9/11/2006 8:00         18.91         6.84         5.89         0.125         0.09         0.192         73.6           9/11/2006 8:15         18.94         6.75         5.89         0.125         0.09         0.192         72.7           9/11/2006 8:30         18.85         6.71         5.9         0.125         0.09         0.192         72.7           9/11/2006 8:45         18.84         6.64         5.9         0.125         0.09         0.192         74.7           9/11/2006 9:10         18.86         6.95         5.9         0.125         0.09         0.192         74.7           9/11/2006 9:15         18.91         7.05         5.9         0.125         0.09         0.192         77.3           9/11/2006 9:45         18.94         7.31         5.89         0.125         0.09         0.192         78.7           9/11/2006 10:01         19         7.45         5.89         0.125         0.09         0.192	9/11/2006 7:15	18.88	6.68	5.89	0.125	0.09	0.192	71.9
9/11/2006 7:45       18.86       6.75       5.9       0.125       0.09       0.192       72.6         9/11/2006 8:00       18.91       6.84       5.89       0.125       0.09       0.192       73.6         9/11/2006 8:15       18.94       6.75       5.89       0.125       0.09       0.192       72.7         9/11/2006 8:30       18.85       6.71       5.9       0.125       0.09       0.192       72.2         9/11/2006 9:00       18.86       6.95       5.9       0.125       0.09       0.192       74.7         9/11/2006 9:00       18.86       6.95       5.9       0.125       0.09       0.192       75.9         9/11/2006 9:30       18.88       7.18       5.9       0.125       0.09       0.192       77.3         9/11/2006 9:30       18.88       7.18       5.9       0.125       0.09       0.192       78.7         9/11/2006 10:00       19       7.45       5.89       0.125       0.09       0.192       78.7         9/11/2006 10:01       19       7.45       5.89       0.125       0.09       0.192       88.7         9/11/2006 10:30       19.16       7.82       5.87       0.125	9/11/2006 7:30	18.9	6.71	5.89	0.125	0.09	0.192	72.2
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	9/11/2006 7:45	18.86	6.75	5.9	0.125	0.09	0.192	72.6
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	9/11/2006 8:00	18.91	6.84	5.89	0.125	0.09	0.192	73.6
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	9/11/2006 8:15	18.94	6.75	5.89	0.125	0.09	0.192	72.7
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	9/11/2006 8:30	18.85	6.71	5.9	0.125	0.09	0.192	72.2
9/11/2006 9:0018.866.955.90.1250.090.19274.79/11/2006 9:1518.917.055.90.1250.090.19275.99/11/2006 9:3018.887.185.90.1250.090.19277.39/11/2006 9:4518.947.315.890.1250.090.19278.79/11/2006 10:00197.455.890.1250.090.19280.39/11/2006 10:1519.097.75.870.1250.090.19283.29/11/2006 10:3019.167.825.870.1250.090.19284.69/11/2006 10:4519.257.885.850.1250.090.19285.49/11/2006 11:1019.317.875.840.1250.090.19285.59/11/2006 11:1319.277.875.860.1250.090.19285.39/11/2006 11:3019.277.875.860.1250.090.19285.39/11/2006 12:0019.277.895.860.1250.090.19285.39/11/2006 12:1519.277.895.860.1250.090.19285.39/11/2006 12:3019.38.145.860.1250.090.19288.3	9/11/2006 8:45	18.84	6.64	5.9	0.125	0.09	0.192	71.4
9/11/2006 9:15         18.91         7.05         5.9         0.125         0.09         0.192         75.9           9/11/2006 9:30         18.88         7.18         5.9         0.125         0.09         0.192         77.3           9/11/2006 9:45         18.94         7.31         5.89         0.125         0.09         0.192         78.7           9/11/2006 10:00         19         7.45         5.89         0.125         0.09         0.192         80.3           9/11/2006 10:15         19.09         7.7         5.87         0.125         0.09         0.192         83.2           9/11/2006 10:30         19.16         7.82         5.87         0.125         0.09         0.192         84.6           9/11/2006 11:45         19.25         7.88         5.85         0.125         0.09         0.192         85.4           9/11/2006 11:00         19.31         7.87         5.84         0.125         0.09         0.192         85.5           9/11/2006 11:13         19.27         7.87         5.86         0.125         0.09         0.192         85.3           9/11/2006 11:45         19.27         7.87         5.86         0.125         0.09         0.192<	9/11/2006 9:00	18.86	6.95	5.9	0.125	0.09	0.192	74.7
9/11/2006 9:30         18.88         7.18         5.9         0.125         0.09         0.192         77.3           9/11/2006 9:45         18.94         7.31         5.89         0.125         0.09         0.192         78.7           9/11/2006 10:00         19         7.45         5.89         0.125         0.09         0.192         80.3           9/11/2006 10:15         19.09         7.7         5.87         0.125         0.09         0.192         83.2           9/11/2006 10:30         19.16         7.82         5.87         0.125         0.09         0.192         84.6           9/11/2006 11:45         19.25         7.88         5.85         0.125         0.09         0.192         85.4           9/11/2006 11:00         19.31         7.87         5.84         0.125         0.09         0.192         85.5           9/11/2006 11:15         19.3         7.88         5.85         0.125         0.09         0.192         85.3           9/11/2006 11:30         19.27         7.87         5.86         0.125         0.09         0.192         85.3           9/11/2006 11:45         19.27         7.89         5.86         0.125         0.09         0.192	9/11/2006 9:15	18.91	7.05	5.9	0.125	0.09	0.192	75.9
9/11/2006 9:45         18.94         7.31         5.89         0.125         0.09         0.192         78.7           9/11/2006 10:00         19         7.45         5.89         0.125         0.09         0.192         80.3           9/11/2006 10:15         19.09         7.7         5.87         0.125         0.09         0.192         83.2           9/11/2006 10:30         19.16         7.82         5.87         0.125         0.09         0.192         84.6           9/11/2006 11:45         19.25         7.88         5.85         0.125         0.09         0.192         85.4           9/11/2006 11:00         19.31         7.87         5.84         0.125         0.09         0.192         85.4           9/11/2006 11:15         19.3         7.88         5.85         0.125         0.09         0.192         85.3           9/11/2006 11:30         19.27         7.87         5.86         0.125         0.09         0.192         85.3           9/11/2006 11:45         19.27         7.87         5.86         0.125         0.09         0.192         85.3           9/11/2006 12:10         19.27         7.89         5.86         0.125         0.09         0.1	9/11/2006 9:30	18.88	7.18	5.9	0.125	0.09	0.192	77.3
9/11/2006 10:00         19         7.45         5.89         0.125         0.09         0.192         80.3           9/11/2006 10:15         19.09         7.7         5.87         0.125         0.09         0.192         83.2           9/11/2006 10:30         19.16         7.82         5.87         0.125         0.09         0.192         84.6           9/11/2006 10:45         19.25         7.88         5.85         0.125         0.09         0.192         85.4           9/11/2006 11:00         19.31         7.87         5.84         0.125         0.09         0.192         85.4           9/11/2006 11:15         19.3         7.88         5.85         0.125         0.09         0.192         85.5           9/11/2006 11:30         19.27         7.87         5.86         0.125         0.09         0.192         85.3           9/11/2006 11:45         19.27         7.87         5.86         0.125         0.09         0.192         85.3           9/11/2006 11:45         19.27         7.87         5.86         0.125         0.09         0.192         85.3           9/11/2006 12:15         19.27         7.89         5.86         0.125         0.09         0.	9/11/2006 9:45	18.94	7.31	5.89	0.125	0.09	0.192	78.7
9/11/2006 10:15         19.09         7.7         5.87         0.125         0.09         0.192         83.2           9/11/2006 10:30         19.16         7.82         5.87         0.125         0.09         0.192         84.6           9/11/2006 10:45         19.25         7.88         5.85         0.125         0.09         0.192         85.4           9/11/2006 11:00         19.31         7.87         5.84         0.125         0.09         0.192         85.4           9/11/2006 11:15         19.3         7.88         5.85         0.125         0.09         0.192         85.5           9/11/2006 11:30         19.27         7.87         5.86         0.125         0.09         0.192         85.3           9/11/2006 11:45         19.27         7.87         5.86         0.125         0.09         0.192         85.3           9/11/2006 11:45         19.27         7.87         5.86         0.125         0.09         0.192         85.6           9/11/2006 12:15         19.27         7.89         5.86         0.125         0.09         0.192         85.6           9/11/2006 12:15         19.27         8         5.86         0.125         0.09         0.	9/11/2006 10:00	19	7.45	5.89	0.125	0.09	0.192	80.3
9/11/2006 10:30         19.16         7.82         5.87         0.125         0.09         0.192         84.6           9/11/2006 10:45         19.25         7.88         5.85         0.125         0.09         0.192         85.4           9/11/2006 11:00         19.31         7.87         5.84         0.125         0.09         0.192         85.4           9/11/2006 11:15         19.3         7.88         5.85         0.125         0.09         0.192         85.4           9/11/2006 11:15         19.3         7.88         5.85         0.125         0.09         0.192         85.5           9/11/2006 11:30         19.27         7.87         5.86         0.125         0.09         0.192         85.3           9/11/2006 11:45         19.27         7.87         5.86         0.125         0.09         0.192         85.3           9/11/2006 12:10         19.27         7.89         5.86         0.125         0.09         0.192         85.6           9/11/2006 12:15         19.27         8         5.86         0.125         0.09         0.192         86.8           9/11/2006 12:30         19.3         8.14         5.86         0.124         0.09         0.1	9/11/2006 10:15	19.09	7.7	5.87	0.125	0.09	0.192	83.2
9/11/2006 10:45         19.25         7.88         5.85         0.125         0.09         0.192         85.4           9/11/2006 11:00         19.31         7.87         5.84         0.125         0.09         0.192         85.4           9/11/2006 11:15         19.3         7.88         5.85         0.125         0.09         0.192         85.5           9/11/2006 11:30         19.27         7.87         5.86         0.125         0.09         0.192         85.3           9/11/2006 11:45         19.27         7.87         5.86         0.125         0.09         0.192         85.3           9/11/2006 12:00         19.27         7.87         5.86         0.125         0.09         0.192         85.3           9/11/2006 12:00         19.27         7.89         5.86         0.125         0.09         0.192         85.6           9/11/2006 12:15         19.27         8         5.86         0.125         0.09         0.192         86.8           9/11/2006 12:30         19.3         8.14         5.86         0.124         0.09         0.192         88.3	9/11/2006 10:30	19.16	7.82	5.87	0.125	0.09	0.192	84.6
9/11/2006 11:00         19.31         7.87         5.84         0.125         0.09         0.192         85.4           9/11/2006 11:15         19.3         7.88         5.85         0.125         0.09         0.192         85.5           9/11/2006 11:30         19.27         7.87         5.86         0.125         0.09         0.192         85.3           9/11/2006 11:45         19.27         7.87         5.86         0.125         0.09         0.192         85.3           9/11/2006 12:00         19.27         7.89         5.86         0.125         0.09         0.192         85.6           9/11/2006 12:15         19.27         7.89         5.86         0.125         0.09         0.192         85.6           9/11/2006 12:15         19.27         8         5.86         0.125         0.09         0.192         86.8           9/11/2006 12:30         19.3         8.14         5.86         0.124         0.09         0.192         88.3	9/11/2006 10:45	19.25	7.88	5.85	0.125	0.09	0.192	85.4
9/11/2006 11:15         19.3         7.88         5.85         0.125         0.09         0.192         85.5           9/11/2006 11:30         19.27         7.87         5.86         0.125         0.09         0.192         85.3           9/11/2006 11:45         19.27         7.87         5.86         0.125         0.09         0.192         85.3           9/11/2006 12:00         19.27         7.89         5.86         0.125         0.09         0.192         85.6           9/11/2006 12:15         19.27         7.89         5.86         0.125         0.09         0.192         85.6           9/11/2006 12:15         19.27         8         5.86         0.125         0.09         0.192         86.8           9/11/2006 12:30         19.3         8.14         5.86         0.124         0.09         0.192         88.3	9/11/2006 11:00	19.31	7.87	5.84	0.125	0.09	0.192	85.4
9/11/2006 11:30         19.27         7.87         5.86         0.125         0.09         0.192         85.3           9/11/2006 11:45         19.27         7.87         5.86         0.125         0.09         0.192         85.3           9/11/2006 12:00         19.27         7.89         5.86         0.125         0.09         0.192         85.6           9/11/2006 12:15         19.27         8         5.86         0.125         0.09         0.192         85.6           9/11/2006 12:15         19.27         8         5.86         0.125         0.09         0.192         86.8           9/11/2006 12:30         19.3         8.14         5.86         0.124         0.09         0.192         88.3	9/11/2006 11:15	19.3	7.88	5.85	0.125	0.09	0.192	85.5
9/11/2006 11:45         19.27         7.87         5.86         0.125         0.09         0.192         85.3           9/11/2006 12:00         19.27         7.89         5.86         0.125         0.09         0.192         85.6           9/11/2006 12:15         19.27         8         5.86         0.125         0.09         0.192         85.6           9/11/2006 12:30         19.3         8.14         5.86         0.124         0.09         0.192         88.3	9/11/2006 11:30	19.27	7.87	5.86	0.125	0.09	0.192	85.3
9/11/2006 12:00         19.27         7.89         5.86         0.125         0.09         0.192         85.6           9/11/2006 12:15         19.27         8         5.86         0.125         0.09         0.192         86.8           9/11/2006 12:30         19.3         8.14         5.86         0.124         0.09         0.192         88.3	9/11/2006 11:45	19.27	7.87	5.86	0.125	0.09	0.192	85.3
9/11/2006 12:15         19.27         8         5.86         0.125         0.09         0.192         86.8           9/11/2006 12:30         19.3         8.14         5.86         0.124         0.09         0.192         88.3	9/11/2006 12:00	19.27	7.89	5.86	0.125	0.09	0.192	85.6
9/11/2006 12:30 19.3 8.14 5.86 0.124 0.09 0.192 88.3	9/11/2006 12:15	19.27	8	5.86	0.125	0.09	0.192	86.8
9/11/2006 12:30 19.3 8.14 5.86 0.124 0.09 0.192 88.3								
	9/11/2006 12:30	19.3	8.14	5.86	0.124	0.09	0.192	88.3

9/11/2006 12:45	19.3	8.25	5.86	0.125	0.09	0.192	89.6
9/11/2006 13:00	19.28	8.28	5.86	0.125	0.09	0.192	89.8
9/11/2006 13:15	19.27	8.29	5.85	0.125	0.09	0.192	89.9
9/11/2006 13:30	19.27	8.28	5.86	0.124	0.09	0.192	89.8
9/11/2006 13:45	19.27	8.24	5.86	0.125	0.09	0.192	89.3
9/11/2006 14:00	19.28	8.18	5.86	0.124	0.09	0.191	88.7
9/11/2006 14:15	19.25	7.98	5.86	0.125	0.09	0.192	86.5
9/11/2006 14:30	19.24	7.77	5.86	0.125	0.09	0.192	84.3
9/11/2006 14:45	19.23	7.65	5.86	0.125	0.09	0.192	82.9
9/11/2006 15:00	19.22	7.5	5.86	0.125	0.09	0.192	81.2
9/11/2006 15:15	19.21	7.23	5.86	0.125	0.09	0.192	78.3
9/11/2006 15:30	19.2	7.12	5.86	0.125	0.09	0.192	77.1
9/11/2006 15:45	19.2	6.65	5.84	0.125	0.09	0.192	72
9/11/2006 16:00	19.19	6.74	5.83	0.125	0.09	0.193	72.9
9/11/2006 16:15	19.2	5.83	5.82	0.126	0.09	0.193	63.1
9/11/2006 16:30	19.19	5.62	5.8	0.126	0.09	0.194	60.8
9/11/2006 16:45	19.19	5.49	5.8	0.126	0.09	0.194	59.4
9/11/2006 17:00	19.18	5.03	5.77	0.127	0.09	0.195	54.5
9/11/2006 17:15	19.18	4.33	5.72	0.128	0.09	0.197	46.9
9/11/2006 17:30	19.18	3.62	5.68	0.129	0.09	0.198	39.2
9/11/2006 17:45	19.19	3.97	5.66	0.129	0.09	0.199	42.9
9/11/2006 18:00	19.19	3.84	5.66	0.129	0.09	0.199	41.6
9/11/2006 18:15	19.2	3.91	5.66	0.129	0.09	0.199	42.4
9/11/2006 18:30	19.21	3.97	5.66	0.129	0.09	0.199	43
9/11/2006 18:45	19.23	4.05	5.69	0.128	0.09	0.197	43.9
9/11/2006 19:00	19.24	4.5	5.8	0.126	0.09	0.194	48.8
9/11/2006 19:15	19.27	6.51	5.8	0.126	0.09	0.194	70.6
9/11/2006 19:30	19.28	6.47	5.79	0.126	0.09	0.194	70.2
9/11/2006 19:45	19.28	6.16	5.76	0.127	0.09	0.195	66.8
9/11/2006 20:00	19.3	6.05	5.75	0.127	0.09	0.195	65.6
9/11/2006 20:15	19.29	5.89	5.75	0.127	0.09	0.195	63.9
9/11/2006 20:30	19.34	6.89	5.78	0.126	0.09	0.194	74.8
9/11/2006 20:45	19.39	7.61	5.8	0.126	0.09	0.193	82.7
9/11/2006 21:00	19.47	7.41	5.78	0.126	0.09	0.193	80.7
9/11/2006 21:15	19.51	7.72	5.79	0.125	0.09	0.193	84.1
9/11/2006 21:30	19.53	7.84	5.79	0.125	0.09	0.193	85.4
9/11/2006 21:45	19.55	7.93	5.79	0.125	0.09	0.193	86.4
9/11/2006 22:00	19.56	8.06	5.79	0.125	0.09	0.193	87.9
9/11/2006 22:15	19.55	8.1	5.79	0.125	0.09	0.193	88.3
9/11/2006 22:30	19.54	8.09	5.8	0.125	0.09	0.193	88.2
9/11/2006 22:45	19.54	8.08	5.8	0.125	0.09	0.193	88.1
9/11/2006 23:00	19.52	7.98	5.8	0.125	0.09	0.193	86.9
9/11/2006 23:15	19.48	7.91	5.8	0.125	0.09	0.193	86.2
9/11/2006 23:30	19.44	7.86	5.81	0.125	0.09	0.193	85.5
9/11/2006 23:45	19.39	7.78	5.81	0.125	0.09	0.193	84.6

## **Appendix B. PHREEQC Files**

#### **B-1:** Partial input file for Example 9 (Parkhurst and Appelo 1999)

TITLE Example 9.--Kinetically controlled oxidation of ferrous iron. # Decoupled valence states of iron. SOLUTION\_MASTER\_SPECIES Fe\_di+2 0.0 Fe\_di Fe\_di 55.847 0.0 Fe\_tri Fe\_tri+3 Fe\_tri 55.847 SOLUTION\_SPECIES  $Fe_di+2 = Fe_di+2$ log\_k 0.0 Fe\_tri+3 = Fe\_tri+3 log\_k 0.0 # # Fe+2 species #  $Fe_di+2 + H2O = Fe_diOH+ + H+$ log\_k -9.5 delta\_h 13.20 kcal # #... and also other Fe+2 species # # # Fe+3 species #  $Fe_{tri+3} + H2O = Fe_{triOH+2} + H+$ log\_k -2.19 delta\_h 10.4 kcal # #... and also other Fe+3 species # PHASES Goethite Fe\_triOOH + 3 H+ = Fe\_tri+3 + 2 H2O log\_k -1.0 END SOLUTION 1 pH 7.0 pe 10.0 O2(g) -0.67 .1 Fe\_di 0.1 Na 10. Cl 10. charge EQUILIBRIUM\_PHASES 1 -0.67 02(g) RATES Fe\_di\_ox -start 10 Fe\_di = TOT("Fe\_di")
20 if (Fe\_di <= 0) then goto 200
30 p\_02 = 10^(SI("02(g)"))
40 molect (200)</pre> 40 moles = (2.91e-9 + 1.33e12 \* (ACT("OH-"))^2 \* p\_o2) \* Fe\_di \* TIME 200 SAVE moles -end KINETICS 1 Fe\_di\_ox

-formula Fe\_di -1.0 Fe\_tri 1.0 -steps 100 400 3100 10800 21600 5.04e4 8.64e4 1.728e5 1.728e5 1.728e5 1.728e5 INCREMENTAL\_REACTIONS true SELECTED\_OUTPUT -file ex9.sel -reset false USER\_PUNCH -headings Days Fe(2) Fe(3) pH si\_goethite 10 PUNCH SIM\_TIME/3600/24 TOT("Fe\_di")\*1e6, TOT("Fe\_tri")\*1e6, -LA("H+"), SI("Goethite") END

#### **B-2: Mantua PHREEQC model complete input and output file**

Input file: F Output file: Database file	F:\Thesis\Kinetics17.j F:\Thesis\Kinetics17 Hesis\Kinetics17 E:\Program Files\U	pqi .pqp SGS\Phreeqt	: Intera	ctive 2.12.5\phreeqc.dat
Reading data	base.			
	SOLUTION MASTER, SHE SOLUTION, SHETES HASES EXCHANCE MASTER, SHE BOLHANGE, SHETES SURFACE, MASTER, SHET SURFACE, SHETES RATES END	CIES IES		
Reading input	data for simulation	1.		
2.12.5\phreed	DAIABASE E:\Program p.dat TIILE Example 9.—K	 Files\USGS inetically	\Phreeq cantrol.	c Interactive led oxidation of ferrous
55.045	ii SOLUTION_MASTER_SPEC Fe_di I	ron. Decoup CIES Fe_di+2	oled vale 0.0	moe states of iron. Fe_di
55.847	Fe_tri I	Fe_tri+3	0.0	Fe_tri
55.847	Fe_tri I SOUTTON_SHELTES Fe_dit-2 = Fe_dit-2 Fe_dit-2 = Fe_dit-3 Fe_dit-2 = Fe_tri-3 Fe_dit-2 + Fe_tri-3 Fe_dit-2 + H20 = Fe_tri-3 Fe_dit-2 + H20 = Fe_tri-3 Fe_dit-2 + H20 = Fe_tri-3 Fe_dit-2 + H20 = Fe_tri-3 Fe_dit-2 + H304 = FR Log_k & 2.2 dalta_h 3.2 Fe_dit-2 + H304 = FR Log_k & 2.2 dalta_h 3.6 Fe_dit-2 + H204 = I Log_k & 2.7 Fe_dit-2 + H204 = I Log_k & 2.7 Fe_dit-2 + H204 = I Log_k & 2.7 Fe_dit-2 + H204 = I Log_k & 2.7 dalta_h 10.7 Fe_tri+3 + H20 = Fe Log_k & -2.7 dalta_h 10.7 Fe_tri+3 + 2 H20 = I Log_k & -2.7 dalta_h 13.1 2 Fe_tri+3 + 2 H20 = I Log_k & -2.7 dalta_h 13.1 2 Fe_tri+3 + 2 H20 = I Log_k & -2.7 dalta_h 13.1 2 Fe_tri+3 + 2 H20 = I Log_k & -2.7 dalta_h 13.1 2 Fe_tri+3 + 2 H20 = I Log_k & -2.7 dalta_h 13.5 Fe_tri+3 + 4 H20 = I Log_k & -2.7 dalta_h 13.5 Fe_tri+3 + 2 H20 = I Log_k & -2.7 dalta_h 13.5 Fe_tri+3 + 4 H20 = I Log_k & -2.7 Fe_tri+3 + H204 = I Log_k & -2.7 Fe_tri+3 + H2	ii(iII+ + II+           ii(iII+ + II+           20         kcal           ii(II)         ii(II)           ii(II)         ii(II)           ii(II)         ii(II)           ii(II)         ii(II)           a.ditRO3+         a.ditRO3+           iF+         trai(H)           trai(H)         4           kcal         re_tri(CH)           s         kcal           s         kcal           if cal         ii(E)           if cal         ii(E)           if cal         ii(CH)           if cal         ii(CH)           ii(CH)         ii(CH)<	0.0 H+ + + 2 H + + 3 H+ + + 3 H+ H)2+4 + H)4+5 + 2 2 4)2 + 4 4+2	Fe_tri + 2 II+ 4 II+
	Fe_tri+3 + 2 F- = Fe log_k 10.8 delta_h 4.8	e_triF2+ 8 kcal		
	re_tr+s + 3 F- = F6 log_k 14.( delta_h 5.4 EQUILIERIUM_PHASES 3 Fe(CH)3(a) 0 10	e_urur3 0 kcal 3		
	END			

Example 9.—Kinetically controlled oxidation of ferrous iron. Decoupled valence states of iron. End of simulation. Reading input data for simulation 2. SOLUTION 1 N 1 pH 4.55 pe -0.924 (2c (g) -0.785 Fe ci 0.161 Na 0.4183 Cl 0.3216 charge Mg 0.9719 Mn 0.0003951 Ca 147.6 Alkalinity 29.67 c 138.9 S 15.79 RTUM HHSES 1 EQUILIBRIUM\_PHASES 1 02 (g) -0.785 C2 (g) -0.785 Fe\_di\_cx start 10 Fe\_di = TOT("Fe\_di") 20 if (Fe\_di <= 0) then goto 200 30 p\_c2 = 10^{+}CS("C2(g)")) 40 moles = (2.91e-9 + 4el3 \* (ACT("CH-"))^2 \* p\_c2) \* Fe\_di \* , مريع مر ۲۹ مرد ۲۹ مر TIME Beginning of initial solution calculations. Initial solution 1. pH will be adjusted to obtain desired alkalinity. -----Solution composition--Elements Molality Moles 2.967e-002 2.967e-002 1.389e-001 1.389e-001 1.476e-001 1.476e-001 2.367e-001 2.367e-001 Charge balance Alkalinity C Ca Cl Cl Fe\_di K Mg Mn 1.610e-004 5.270e-005 5.270e-005 5.270e-005 9.719e-004 9.719e-004 3.951e-007 3.951e-007 Na S 4.183e-004 4.183e-004 1.579e-002 1.579e-002 --Description of solution--Adjust alkalinity Equilibrium with pH = 5.434 pe = 15.168 02 (g) C2(g) Activity of water = 0.991 Ionic strength = 4.068e-001 Mass of water (kg) = 1.000e+000 Total C02 (mOl/kg) = 1.3398-001 Temperature (deg C) = 25.000 Electrical balance (eg) = -3.112e-015 Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.00 Iterations = 19 Total H = 1.110421e+002 Total O = 5.587722e+001 -Distribution of species Log Log Log Species Molality Activity Molality Activity Ganna 4.766e-006 3.678e-006 -5.322 -5.434 H+ -0.113 OH-4.154e-009 2.698e-009 -8.382 -8.569 -0.187 H2O 5.551e+001 9.911e-001 1.744 -0.004 0.000 C(-4) 0.000e+000 CH4 0.000e+000 0.000e+000 -141.384 -141.344 0.041 C(4) 1.389e-001

0.041	CC2	1.092e-001	1.200e-001	-0.962	-0.921
0.041	HC03-	2.043e-002	1.438e-002	-1.690	-1.842
-0.152	CaHCO3+	9.116e-003	6.417e-003	-2.040	-2.193
-0.152	MaHCO3+	5.781e-005	4.225e-005	-4.238	-4.374
-0.136	Fe diHCO3+	5.274e-005	3.854e-005	-4.278	-4.414
-0.136	രന്ദ	9 811-006	1 077-005	-5.008	_/ 968
0.041		2.172-000	2.200000	-5.000	-4.500
0.041	Nahuos	2.172e-006	2.3800-000	-5.005	-3.022
-0.610	03-2	/.4666-007	1.8340-007	-6.12/	-6./3/
0.041	Fe_diC03	1.0/4e-00/	1.1/9e-00/	-6.969	-6.928
-0.136	MnHCO3+	1.037e-007	7.582e-008	-6.984	-7.120
0.041	MgCO3	4.001e-008	4.394e-008	-7.398	-7.357
-0.136	NaCO3-	1.378e-009	1.007e-009	-8.861	-8.997
0.041	MnCO3	7.846e-010	8.617e-010	-9.105	-9.065
Ca	1.476e-001	1 2030 001	3 /090 002	0 999	1 456
-0.568	G 72	0.010.000	1 010 000	-0.005	-1.400
0.041	Ca304	9.212e-003	1.012e-002	-2.036	-1.995
-0.152	Carcos+	9.116e-003	6.417e-003	-2.040	-2.193
0.041	CaCO3	9.811e-006	1.07/e-005	-5.008	-4.968
-0.136	CaHSO4+	2.982e-007	2.180e-007	-6.525	-6.662
-0.136	CaCH+	2.141e-009	1.565e-009	-8.669	-8.806
Cl	2.367e-001	2.367e-001	1.559e-001	-0.626	-0.807
-0.181	Te dicl+	7 893-006	5 768-006	_5 103	_5 239
-0.136	Necl.	F 1410 000	2 7570 000	7 200	7 405
-0.136	MCI+	0.000 000	3.737e-000	-7.209	-7.420
0.041	MhC12	2.3280-009	2.55/e-009	-8.633	-8.592
-0.136	MhCL3-	1.502e-010	1.098e-010	-9.823	-9.960
Fe_di	1.610e-004 Fe_di+2	9.396e-005	2.681e-005	-4.027	-4.572
-0.545	Fe diHCO3+	5.274e-005	3.854e-005	-4.278	-4.414
-0.136	Fe diCl+	7.893e-006	5.768e-006	-5.103	-5.239
-0.136	Fe dig04	6 292-006	6 909-006	-5 201	-5 161
0.041	Fo dima	1 0740 007	1 1796 007	6 969	6 979
0.041	To dictu	2 126- 000	2 2940 000	0.505	0.520
-0.136	Pe_dium	3.120e-009	2.204C-009	-0.000	-0.041
-0.136	Fe_diH504+	2.2850-010	1.6/08-010	-9.041	-9.///
0.041	Fe_di(HS)2	0.000e+000	0.000e+000	-2/4.519	-2/4.4/9
-0.136	Fe_di (HS)3-	0.000e+000	0.000e+000	-411.734	-411.870
H(0)	0.000e+000 H2	0.000e+000	0.000e+000	-44.396	-44.355
0.041 K	5.270e-005				
-0.181	K+	5.222e-005	3.439e-005	-4.282	-4.464
_0 136	K904-	4.793e-007	3.503e-007	-6.319	-6.456
0.041	KOH	2.927e-014	3.214e-014	-13.534	-13.493
Mg	9.719e-004	0.264004	0 511- 004	2 070	3 (00
-0.523	Mg+2	8.3040-004	2.5110-004	-3.078	-3.600
0.041	MgSO4	7.770e-005	8.532e-005	-4.110	-4.069
-0.136	MgHCO3+	5.781e-005	4.225e-005	-4.238	-4.3/4
0.041	MgCO3	4.001e-008	4.394e-008	-7.398	-7.357
-0.136	MgCH+	3.362e-010	2.457e-010	-9.473	-9.610
Mn(2)	3.951e-007 Mn+2	2.228e-007	5.916e-008	-6.652	-7.228
-0.576	MoHOOR+	1 037-007	7 582-008	_6.984	_7 120
-0.136	Macily	E 141- 000	2 7570 000	7 200	7 405
-0.136	MLI+	1 200- 000	1 525- 000	-7.209	-7.420
0.041	M1504	1.3890-008	1.5258-008	-/.85/	-/.81/
0.041	MINULZ	2.328e-009	2.55/e-009	-8.633	-8.592
0.041	MnCO3	7.846e-010	8.617e-010	-9.105	-9.065
-0.136	MnCl3-	1.502e-010	1.098e-010	-9.823	-9.960
-0.136	MhOH+	5.608e-013	4.098e-013	-12.251	-12.387
Mn(3)	4.528e-017 Mn+3	4.528-017	2.693e-018	-16.344	-17,570
-1.226	4 1830 004			10.011	1
0.146	4.1002-004 Na+	4.132e-004	2.950e-004	-3.384	-3.530
-0.120	Na904-	2.933e-006	2.143e-006	-5.533	-5.669
0.041	NaHCO3	2.172e-006	2.386e-006	-5.663	-5.622
0.041	NaCO3-	1.378e-009	1.007e-009	-8.861	-8.997
0 100					

0.041	NaCH	4.784e-013	5.253e-013	-12.320	-12.280
0.041 O(0)	3.828e-004	1.914e-004	2.102e-004	-3.718	-3.677
0.041 S(-2)	0.000e+000	0.000-1000	0.000000	127.002	107 001
0.041	H2S	0.000e+000	0.000e+000	-137.962	-137.921
-0.187	H5-	0.000=+000	0.000=.000	-139.241	-139.429
-0.635	5-2 To di (TC\)	0.000e+000	0.000e+000	-140.277	-140.912
0.041	Fe_di (HS) 3_	0.000e+000	0.000e+000	-214.019	-214.475
-0.136 S(6)	1.579e-002	010000.000	010000.000		1111070
0.041	Ca904	9.212e-003	1.012e-002	-2.036	-1.995
-0.651	SO4-2	6.490e-003	1.449e-003	-2.188	-2.839
0.041	MgSO4	7.770e-005	8.532e-005	-4.110	-4.069
0.041	Fe_diSO4	6.292e-006	6.909e-006	-5.201	-5.161
-0.136	NaSO4-	2.933e-006	2.143e-006	-5.533	-5.669
-0.136	HSO4-	7.091e-007	5.183e-007	-6.149	-6.285
-0.136	K904-	4.793e-007	3.503e-007	-6.319	-6.456
-0.136	Cars04+	2.982e-007	2.180e-007	-0.525	-0.662
0.041	MISO4	2.205- 010	1.5250-008	-/.85/	-7.817
-0.136	Fe_QIH504+	2.2858-010	1.6/08-010	-9.041	-9.111
		Saturation i	ndices		
	Phase	SI log I	AP log KT		
	Anhydrite Aragonite Calcite	0.07 -4.1 0.14 -8.1 0.29 -8	29 -4.36 19 -8.34 19 -8.48	CaSO4 CaCO3 CaCO3	
	CH4 (g) (02 (a)	-138.48 -141.3	34 -2.86 32 -1.47	CH4 (1)2	
	Dolomite Gypsun	-1.44 -18. 0.28 -4.	53 -17.09 30 -4.58	CaMg(003)2 CaS04:2H20	
	H2 (g) H2O(a)	-41.21 -44.3	36 -3.15 00 1.51	H2 H2O	
	H2S(g) Halite	-136.92 -137.9	92 -1.00 34 1.58	H2S NaCl	
	Hausmannite Manganite	-8.92 52. -1.10 24.1	11 61.03 24 25.34	Min3O4 MinOCH	
	02(g) Pvrochroite	-0.78 -3.0	58 -2.89 53 15.20	02 Mn (OH) 2	
	Pyrolusite Rhodochrosite	3.46 44.1 -2.83 -13.9	84 41.38 96 -11.13	MhO2 MhO03	
	Sulfur	-101.60 -96.	72 4.88	S	
Beginning of	batch-reaction	calculations.			
Reaction ste	p1.				
Using solutio	on 1. hase assemblace	1.			
Using kinetio	as 1.	Kinetics define	ed in simula	ation 2.	
Kinetics 1.	Kinetics defir	ed in simulatio	m 2.		
	Time step: 100 Rate name	) seconds (Inc. Delta Moles /	remented ti Ibtal Moles	me: 100 sec Reactant	ands)
Coefficient	Time step: 100 Rate name	) seconds (Inc. Delta Moles '	remented ti Iotal Moles	me: 100 sec Reactant	ands)
Coefficient -1	Time step: 100 Rate name Fe <u>di</u> ox	) seconds (Inc. Delta Moles ? -7.679e-007	remented ti Iotal Moles 1.000e+000	me: 100 sec Reactant Fe_di	ands)
Coefficient -1 1	Time step: 100 Rate name Fe <u>di</u> ox	) seconds (Inc. Delta Moles ? -7.679e-007	remented ti Iotal Moles 1.000e+000	me: 100 sec Reactant Fe_di Fe_tri	ands)
0xefficient -1 1 	Time step: 100 Rate name Fe_di_ox	) seconds (Inc. Delta Moles ? -7.679e-007 Phase assert	remented ti Iotal Moles 1.000e+000 blage	me: 100 sec Reactant Fe_di Fe_tri 	ands) 
Opefficient -1 1 	Time step: 100 Rate name Fe_di_ox	) seconds (Inc. Delta Moles ' -7.679e-007 Phase assent	remented ti Iotal Moles 1.000e+000 blage	me: 100 sec Reactant Fe_di Fe_tri Moles_in_as	ands) 
Obefficient -1 1 Delta	Time step: 100 Rate name Fe_di_ox Phase	) seconds (Inc: Delta Moles ' -7.679e-007 Phase assent SI log I	remented tin Total Moles 1.000e+000 blage blage	me: 100 sec Reactant Fe_di Fe_tri Fe_tri Moles in as Initial	ands)  sentblage Final
Coefficient -1 1 Delta 1.920e-007	Time step: 100 Rate name Fe_di_ox Fhase G2 (g)	) seconds (Inc: Delta Moles ' -7.679e-007 	remented tin Total Moles 1.000e+000 blage AP log KT 58 -2.89	me: 100 sec Reactant Fe_di Fe_tri Moles in as Initial	ands) semblage Final 1.000e+001-
Coefficient -1 1 Delta 1.920e-007	Time step: 100 Rate name Fe_di_ox Fhase 02 (g)	) seconds (Inc Delta Moles ' -7.679e-007 Phase assent SI log I -0.78 -3.0 Solution comp	remented til Total Moles 1.000e+000 blage AP log KT 58 -2.89 osition	me: 100 sec Reactant Fe_di Fe_tri Moles in as Initial 1.000e+001	ands) semblage Final 1.000e+001-
Coefficient -1 1 Delta 1.920e-007	Time step: 100 Rate name Fe_di_ox Phase 02 (g) Elements	) seconds (Inc Delta Moles ' -7.679e-007 Phase assent SI log L -0.78 -3.0 Solution comp Molality	remented til Total Moles 1.000e+000 blage AP log KT 58 -2.89 csition Moles	me: 100 sec Reactant Pe_di Pe_tri  Moles in as Initial 1.000e+001	ands) semblage Final 1.000e+001-
Coefficient -1 1 Delta 1.920e-007	Time step: 100 Rate name Fe_di_ox Phase (2(g) Elements C	<ul> <li>) seconds (Inc.</li> <li>Delta Moles '</li> <li>-7.679e-007</li> <li>Phase assent</li> <li>SI log I</li> <li>-0.78 -3.</li> <li>-Solution comp</li> <li>Molality</li> <li>1.389e-001</li> </ul>	remented til Iotal Moles 1.000e+000 blage AP log KT 58 -2.89 csition Moles 1.389e-001	me: 100 sec Reactant Fe_di Fe_tri Moles in as Initial 1.000e+001	ands) sentblage Final 1.000e+001-
Coefficient -1 1 Delta 1.920e-007	Time step: 100 Rate name Fe_di_ox Phase 02 (g) Elements C Ca CL	<ul> <li>) seconds (Inc.</li> <li>Delta Moles '</li> <li>-7.679e-007</li> <li>-7.679e-007</li> <li>-7.679e-001</li> <li>Solution comp</li> <li>Molality</li> <li>1.389e-001</li> <li>1.476e-001</li> <li>2.367e-001</li> </ul>	remented til Iotal Moles 1.000e+000 blage AP log KT 58 -2.89 ceition 58 -2.89 ceition Moles 1.383e-001 1.476e-001 2.367e-001	me: 100 sec Reactant Fe_di Fe_tri Moles in as Initial 1.000e+001	ands) semblage Final 1.000e+001-
Coefficient -1 1 Delta 1.920e-007	Time step: 100 Rate name Fe_di_ox Phase 02 (g) Elements C Ca Cl Ci Ci Ci Fe_dii Fe_tri	<ul> <li>Detta Moles '</li> <li>-7.679e-007</li> <li>-7.679e-007</li> <li>-7.679e-007</li> <li>-7.679e-001</li> <li>-0.78</li> <li>-3.1</li> <li>-50lution comp Molality</li> <li>1.389e-001</li> <li>1.476e-001</li> <li>2.367e-001</li> <li>1.602e-004</li> <li>7.679e-007</li> </ul>	remented til Total Moles 1.000e+000 blage blage S8 -2.89 csition Moles 1.339e-001 1.476e-001 2.367e-001 1.602e-004 7.679e-007	me: 100 sec Reactant Fe_di Fe_tri Moles in as Initial 1.000e+001	ands) senblage Final 1.000e+001-
Coefficient -1 1 Delta 1.920e-007	Time step: 100 Rate name Fe_di_ox Fe_di_ox C2 (g) Elements C Ca Ca Ca Ca Ca Ca Ca Ca K K Mg	<ul> <li>Deta Moles '         <ul> <li>-7.679e-007</li> <li>-7.679e-007</li> <li>-7.679e-007</li> <li>SI log I</li> <li>-0.783.0</li> <li>-Solution comp</li> <li>Molality</li> <li>1.399e-001</li> <li>1.676e-001</li> <li>2.567e-001</li> <li>1.676e-001</li> <li>7.679e-001</li> <li>7.679e-001</li> <li>7.679e-001</li> </ul> </li> </ul>	remented til Total Moles 1.000e+000 blage AP log KT 58 -2.89 cosition 1.389e-001 1.476e-001 2.367e-001 1.602e-004 7.679e-007 5.270e-005 9.719e-004	me: 100 sec Reactant Fe_di Fe_tri Moles in as Initial 1.000e+001	ands) semblage Final 1.000e+001-
Coefficient -1 1 Delta 1.920e-007	Time step: 100 Rate name Fe_di_ox Fe_di_ox C2 (g) Elements C Ca C1 Fe_di Fe_tri K Mg Mh Na	<ul> <li>accords (Inc.</li> <li>Delta Moles '</li> <li>-7.679e-007</li> <li>-7.679e-007</li> <li>-7.679e-007</li> <li>SI log I</li> <li>-0.78 -3.0</li> <li>-3.0</li> <li>-3.0</li></ul>	remented til Total Moles 1.000e+000 blage AP log KT 58 -2.89 csition 1.399e-001 1.602e-004 7.679e-007 5.270e-005 9.719e-004 3.951e-007 4.133e-004 4.133e-004	me: 100 sec Reactant Fe_di Fe_tri Moles in as Initial 1.000e+001	ands) sentblage Final 1.000e+001-
Oxefficient -1 1 Delta 1.920e-007	Time step: 100 Rate name Fe_di_ox Fe_di_ox Ehase O2(g) Elements C Ca Cl Ca Cl Ca Cl Ca Cl K Mn Na S	<ul> <li>a) seconds (Inc: Delta Moles ' -7.679e-007</li> <li>-7.679e-007</li> <li>SI log I -0.78 -3.0</li> <li>-3.1</li> <li>-3.1</li></ul>	remented til Total Moles 1.000e+000 blage AP log KT 58 -2.89 csition Moles 1.389e-001 2.367e-001 1.476e-001 2.367e-001 1.602e-004 5.270e-005 9.795e-007 1.579e-002 0.15799e-002 0.1	me: 100 sec Reactant Fe_di Fe_tri Pe_tri Initial	ands) semblage Final 1.000e+001-
Coefficient -1 1 Delta 1.920e-007	Time step: 100 Rate name Fe_di_ox Fe_di_ox Phase 02 (g) Elements C Ca Ca Cl Fe_di Mn Na S	<ul> <li>Decomb (Inc.</li> <li>Delta Moles '</li> <li>-7.679e-007</li> <li>-7.679e-007</li> <li>SI log I</li> <li>-0.78 -3.0</li> <li>-Solution comp</li> <li>Molality</li> <li>1.389e-001</li> <li>1.476e-001</li> <li>2.367e-001</li> <li>3.651e-007</li> <li>3.591e-007</li> <li>4.183e-004</li> <li>4.579e-002</li> <li>Description of</li> </ul>	remented til Total Moles 1.000e+000 blage P log KT 58 -2.89 csittion 1.476e-001 2.367e-001 1.602e-004 9.719e-004 3.951e-007 5.270e-005 9.719e-004 3.951e-007 5.270e-005 9.719e-004 3.951e-007 5.270e-005 9.719e-004 3.951e-007 5.270e-005 9.719e-004 3.951e-007 5.270e-005 9.719e-004 5.270e-005 5.	me: 100 sec Reactant Fe_di Fe_tri Initial 1.000e+001	ands) semblage Final 1.000e+001-
Coefficient -1 1 Delta 1.920e-007	Time step: 100 Rate name Fe_di_ox Fe_di_ox Phase (2 (g) Elements C Ca C1 Fe_di Fe_di Fe_tri Na S	) seconds (Inc Delta Moles ' -7.679e-007 Phase assent SI log I -0.78 -3.0 Solution comp Molality 1.389e-001 1.476e-001 2.367e-001 1.602e-004 3.951e-007 4.1859e-002 1.559e-002 Description of pH pe	remented til Total Moles 1.000e+000 blage AP log KT 58 -2.89 osition 1.476e-001 2.367e-001 1.602e-004 7.679e-07 9.719e-004 3.951e-077 4.183e-004 1.579e-002 solution = 5.434 = 15.148	me: 100 sec Reactant Fe_di Fe_tri Moles in as Initial 1.000e+001	ands) satiblage Final 1.000e+001- 
Coefficient -1 1 Delta 1.920e-007 equilibrium	Time step: 100 Rate name Fe_di_ox Phase (2 (g) Elements C Ca Cl Fe_di Fe_di Fe_tri K Mg Mn Na S	) seconds (Inc. Delta Moles ' -7.679e-007 Phase assemi SI log I -0.78 -3.1 Solution comp Molality 1.389e-001 1.476e-001 2.367e-001 1.602e-004 7.679e-007 5.719e-004 3.951e-007 4.183e-004 1.579e-002 Description of Ph pe	remented til Total Moles 1.000e+000 blage AP log KT 58 -2.89 cosition 1.476e-001 2.367e-001 1.476e-001 2.367e-001 1.602e-004 9.719e-004 1.579e-002 solution = 5.434 = 15.168 = 0.991	me: 100 sec Reactant Fe_di Fe_tri Moles in as Initial 1.000e+001 	ands) semblage Final 1.000e+001- 
Coefficient -1 1 Delta 1.920e-007 equilibrium	Time step: 100 Rate name Fe_di_ox Fe_di_ox Phase 02 (g) Elements C Ca Cl Fe_dii Fe_trii K Mg Mn Na S Act: Mass	<ul> <li>accords (Inc: Delta Moles ' -7.679e-007</li> <li>-7.679e-007</li> <li>SI log I -0.78 -3.1</li> <li>-Solution comp Molality</li> <li>1.389e-001</li> <li>1.476e-001</li> <li>2.367e-001</li> <li>1.602e-004</li> <li>7.679e-007</li> <li>5.719e-004</li> <li>3.951e-007</li> <li>4.183e-004</li> <li>1.579e-002</li> <li>Description of pH pe</li> <li>tity of water foric strength</li> </ul>	AP log KT 58 -2.89 5.362-001 1.476e-001 2.367e-001 1.476e-001 2.367e-001 1.476e-001 2.367e-001 3.951e-007 3.951e-007 3.951e-007 4.183e-004 1.579e-002 solution	me: 100 sec Reactant Fe_di Fe_tri Moles in as Initial 1.000e+001 	ands) semblage Final 1.000e+001- 

	Total alkalin Total C	uity (eg/kg) D2 (mol/kg)	= 2.967e-0 = 1.389e-0	02 01	
	Tenperat Electrical b	ure (deg C) alance (eg)	= 25.000 = -1.008e-0	)14	
Percent erro	or, 100*(Cat- An )	/(Cat+ An ) Iterations	= -0.00 = 41		
		Total H	= 1.110421e	+002	
	Di	ctribution of	= 0.007722e	51001	
	Di	SCIENCIAIC	i species		
_				Log	Log
Log	Species	Molality	Activity	Molality	Activity
Gamma					
-0.113	H+	4.767e-006	3.678e-006	-5.322	-5.434
-0.187	OH-	4.154e-009	2.698e-009	-8.382	-8.569
0.000	H2O	5.551e+001	9.911e-001	1.744	-0.004
C(-4)	0.000e+000 CH4	0.000e+000	0.000e+000	-141.384	-141.344
0.041 C(4)	1 389e-001				
0.041	002	1.092e-001	1.200e-001	-0.962	-0.921
_0 152	H003-	2.043e-002	1.438e-002	-1.690	-1.842
0.152	CaHCO3+	9.116e-003	6.417e-003	-2.040	-2.193
0.126	MgHCO3+	5.781e-005	4.225e-005	-4.238	-4.374
-0.130	Fe_diH003+	5.249e-005	3.836e-005	-4.280	-4.416
-0.130	CaCO3	9.811e-006	1.077e-005	-5.008	-4.968
0.041	NaHCO3	2.172e-006	2.386e-006	-5.663	-5.622
0.041	003-2	7.466e-007	1.833e-007	-6.127	-6.737
-0.610	Fe_di003	1.068e-007	1.173e-007	-6.971	-6.931
0.041	MnHCO3+	1.037e-007	7.582e-008	-6.984	-7.120
-0.136	MgCO3	4.001e-008	4.393e-008	-7.398	-7.357
0.041	NaCO3-	1.378e-009	1.007e-009	-8.861	-8.997
-0.136	Mp(TO3	7.846e-010	8.617e-010	-9.105	-9.065
0.041	1 476-001	10100 010	010170 010	51105	51005
_0 568	Ca+2	1.293e-001	3.498e-002	-0.889	-1.456
0.041	Ca904	9.212e-003	1.012e-002	-2.036	-1.995
0.150	CaHCO3+	9.116e-003	6.417e-003	-2.040	-2.193
0.112	CaCO3	9.811e-006	1.077e-005	-5.008	-4.968
0.041	CaHSO4+	2.982e-007	2.180e-007	-6.525	-6.662
-0.130	CaCH+	2.141e-009	1.564e-009	-8.669	-8.806
-0.136 Cl	2.367e-001				
-0.181	CL-	2.367e-001	1.559e-001	-0.626	-0.807
-0.136	Fe_diCl+	7.855e-006	5.741e-006	-5.105	-5.241
-0.136	MnCl+	5.141e-008	3.757e-008	-7.289	-7.425
0.041	MnCl2	2.328e-009	2.557e-009	-8.633	-8.592
-0.136	MnCl3-	1.502e-010	1.098e-010	-9.823	-9.960
-0.545	Fe <u>tri</u> Cl+2	5.669e-011	1.617e-011	-10.246	-10.791
-0.136	Fe_triCl2+	1.541e-011	1.126e-011	-10.812	-10.948
0.041	Fe_triCl3	1.599e-013	1.756e-013	-12.796	-12.756
Fe_di	1.602e-004 Fe di+2	9.352e-005	2.668e-005	-4.029	-4.574
-0.545	Fe diH003+	5 249-005	3 836-005	-4 280	-4 416
-0.136	Fe diCl+	7.855-006	5.741e-006	-5.105	-5,241
-0.136	Fe dis04	6.262-005	6.876-006	-5 203	-5.163
0.041	Fe dim	1 068- 007	1 172-007		_6 931
0.041	Fe diam	3 1110 000	2 274~ 000	-0.5/1	_8 EV3
-0.136		2 275- 010	1 6620 010	0.00/	-0.0±0
-0.136		2.2750-010	0.000000	-9.045	-9.119
0.041	re_ut(ns)2	0.000.000	0.000.000	-2/4.522	-2/4.481
-0.136	re_ol(HS)3-	v.uuue+000	v.uuue+000	-411.736	-411.8/2
re <u>tri</u>	7.6/9e-00/ Fe_tri (OH) 2+	7.299e-007	5.334e-007	-6.137	-6.273
-0.136	Fe_triOH+2	2.095e-008	5.978e-009	-7.679	-8.223
-0.545	Fe_tri(OH)3	1.686e-008	1.852e-008	-7.773	-7.732
0.041	Fe_triSO4+	7.471e-011	5.460e-011	-10.127	-10.263
-0.136	Fe tri+3	5.776e-011	3.436e-012	-10.238	-11.464
-1.226	Fe triC1+2	5.669e-011	1.617e-011	-10.246	-10,791
-0.545	Fe triCl2+	1.541-011	1.126-011	-10 812	-10.948
-0.136	Fe tri (041/1_	6 228-012	4 551_012	_11 206	_11 3/12
-0.136	<u>-</u>	J.220C-012	210-210-210	41.200	244.144

0 126	Fe_tri(SO4)2-	2.369e-012	1.731e-012	-11.625	-11.762
-0.130	Fe_triCl3	1.599e-013	1.756e-013	-12.796	-12.756
0.041	Fe_tri2(CH)2+4	1.452e-013	9.618e-016	-12.838	-15.017
-2.179	Fe_triH904+2	1.885e-015	5.377e-016	-14.725	-15.269
-0.545	Fe_tri3(CH)4+5	2.721e-016	1.072e-019	-15.565	-18.970
-3.405 H(0)	0.000e+000				
0.041	H2	0.000e+000	0.000e+000	-44.396	-44.355
K	5.270e-005 K+	5.222e-005	3.439e-005	-4.282	-4.464
-0.181	K904-	4 793-007	3 503-007	-6 319	-6 456
-0.136	KOH	2 927-01/	3 21/0-01/	_13 534	_13 /93
0.041 Mr	9 719-004	2.92/0 014	5.2140 014	10:004	10.400
0 523	Mg+2	8.364e-004	2.511e-004	-3.078	-3.600
-0.525	MgSO4	7.770e-005	8.532e-005	-4.110	-4.069
0.041	MgHCO3+	5.781e-005	4.225e-005	-4.238	-4.374
-0.136	MgCO3	4.001e-008	4.393e-008	-7.398	-7.357
0.041	MgCH+	3.362e-010	2.457e-010	-9.473	-9.610
-0.136 Mn(2)	3.951e-007				
-0.576	Min+2	2.228e-007	5.916e-008	-6.652	-7.228
-0.136	MinHCO3+	1.037e-007	7.582e-008	-6.984	-7.120
-0.136	MnCl+	5.141e-008	3.757e-008	-7.289	-7.425
0.041	Min904	1.389e-008	1.525e-008	-7.857	-7.817
0.041	MnCl2	2.328e-009	2.557e-009	-8.633	-8.592
0.041	MhCO3	7.846e-010	8.617e-010	-9.105	-9.065
_0 136	MnCl3-	1.502e-010	1.098e-010	-9.823	-9.960
-0.136	MnOH+	5.608e-013	4.098e-013	-12.251	-12.387
Mn(3)	4.528e-017	4 520- 017	2 602- 010	16 244	17 570
-1.226	4 102 004	4.5208-017	2.0958-010	-10.344	-17.570
Na	4.183e-004 Na+	4.132e-004	2.950e-004	-3.384	-3.530
-0.146	Na904-	2.933e-006	2.143e-006	-5.533	-5.669
-0.136	NaHCO3	2.172e-006	2.386e-006	-5.663	-5.622
0.041	NaCO3-	1.378e-009	1.007e-009	-8.861	-8.997
-0.136	NaCH	4.784e-013	5.253e-013	-12.320	-12.280
0.041 O(0)	3.828e-004				
0.041	02	1.914e-004	2.102e-004	-3.718	-3.677
S(-2)	0.000e+000 H2S	0.000e+000	0.000e+000	-137.962	-137.921
0.041	HS-	0.000e+000	0.000e+000	-139.241	-139,428
-0.187	s-2	0.000e+000	0.000e+000	-146.277	-146.912
-0.635	Fe di (HS)2	0.000e+000	0.000e+000	-274.522	-274.481
0.041	Fe di (HS) 3	0.000e+000	0.000e+000	-411 736	-411 872
-0.136	1 579-002	010002.000	010000-000		11110/2
0.041	Ca904	9.212e-003	1.012e-002	-2.036	-1.995
0.651	SO4-2	6.490e-003	1.449e-003	-2.188	-2.839
-0.0JI	MgSO4	7.770e-005	8.532e-005	-4.110	-4.069
0.041	Fe_diSO4	6.262e-006	6.876e-006	-5.203	-5.163
0.041	Na904-	2.933e-006	2.143e-006	-5.533	-5.669
-0.136	H904-	7.092e-007	5.183e-007	-6.149	-6.285
-0.136	K904-	4.793e-007	3.503e-007	-6.319	-6.456
-0.136	CaHSO4+	2.982e-007	2.180e-007	-6.525	-6.662
-0.136	Mn904	1.389e-008	1.525e-008	-7.857	-7.817
0.041	Fe_diH904+	2.275e-010	1.662e-010	-9.643	-9.779
-0.136	Fe_triSO4+	7.471e-011	5.460e-011	-10.127	-10.263
-0.136	Fe tri (904)2-	2.369e-012	1.731e-012	-11.625	-11.762
-0.136	Fe triHSO4+2	1.885e-015	5.377e-016	-14.725	-15.269
-0.545	·				
		-Saturation i	ndices		
	Phase	ST log T	AP ]oor KTT		
	Anhudrite	0.07 _/	29 _4 36	Ca904	
	Aragonite	0.14 -8.	19 -8.34 19 -8.49	CaCC3	
	CH4 (g) -	-138.48 -141.	34 -2.86 92 _1 /7	CH4 (1)2	
	Dolomite	-1.44 -18.	53 -17.09	CaMg(003)2	
	H2 (g)	-41.21 -44.	36 -3.15		
	H2S(g) -	-136.92 -137.	92 -1.00	H2S	

	Halite	-5.92 -4.2	34 1.58	NaCl		0.041	Ca904	9.212e-003	1.012e-002	-2.036	-1.995
	Manganite	-8.92 52.	24 25.34 1	Mn304 Mn00H		0.041	CaHCO3+	9.115e-003	6.417e-003	-2.040	-2.193
	02(g) Pyrochroite	-0.78 -3.0	68 –2.89 ( 63 15.20 1	02 Min (OH) 2		-0.152	CaCO3	9.809e-006	1.077e-005	-5.008	-4.968
	Pyrolusite Rhodochrosite	3.46 44.1	84 41.38 1 96 -11.13 1	MinCO3		0.041	CaHSO4+	2.983e-007	2.180e-007	-6.525	-6.662
	Sulfur	-101.60 -96.7	72 4.88	S		-0.136	CaOH+	2.140e-009	1.564e-009	-8.669	-8.806
Reaction step	p 2.					-0.136 Cl	2.367e-001				
Using solutio	an 1.	1				0.191	cl-	2.367e-001	1.559e-001	-0.626	-0.807
Using kinetio	cs 1. F	linetics define	ed in simulat	tion 2.		-0.101	Fe_diCl+	7.707e-006	5.632e-006	-5.113	-5.249
Kinetics 1.	Kinetics define	ad in simulatio	an 2.			-0.136	MnCl+	5.141e-008	3.757e-008	-7.289	-7.425
	Time step: 400	seconds (Inc	remented tim	e: 500 sec	rands)	-0.136	MnCl2	2.328e-009	2.557e-009	-8.633	-8.592
	Rate name	Delta Moles '	Total Moles	Reactant	:	0.041	Fe_triCl+2	2.806e-010	8.005e-011	-9.552	-10.097
Coefficient						-0.545	MnCl3-	1.502e-010	1.098e-010	-9.823	-9.959
-1	Fe_di_ax	-3.032e-006	1.000e+000	Fe_di		-0.136	Fe triCl2+	7.627e-011	5.574e-011	-10.118	-10.254
1				Fe <u>t</u> ri		-0.136	Fe triCl3	7 912-013	8 689-013	-12 102	-12 061
-		Phaco accorri	blace			0.041 Fe di	1 572-004		0.0050 015	101100	111001
			Circage			0.646	Fe_di+2	9.175e-005	2.617e-005	-4.037	-4.582
		OT 1 T	M les M	bles in as	senblage	-0.545	Fe_diHCO3+	5.149e-005	3.763e-005	-4.288	-4.424
Delta	Phase	SI log L	AP LOG KI'	Initial	Final	-0.136	Fe_diCl+	7.707e-006	5.632e-006	-5.113	-5.249
	02 (g)	-0.79 -3.0	68 -2.89 1	.000e+001	1.000e+001-	-0.136	Fe_diSO4	6.143e-006	6.746e-006	-5.212	-5.171
7.581e-007						0.041	Fe di003	1.048e-007	1.151e-007	-6.980	-6.939
		-Solution comp	osition			0.041	Fe diOH+	3 052-009	2 230-009	-8 515	-8 652
	Flamanta	Molalitzz	Moloc			-0.136	Fo diugna	2 2320 010	1 6310 010	9 651	0.799
		1 200- 001	1 200- 001			-0.136	Fe_direct+	0.000000	0.000000	-9.001	-9.700
	Ca	1.385e-001	1.476e-001			0.041	Fe_01(HS)2	0.000000000	0.00000000	-274.000	-2/4.409
	Fe_di	2.36/e-001 1.572e-004	2.36/e-001 1.572e-004			-0.136	Fe <u>a</u> t (HS) 3-	0.000e+000	0.0000+000	-411./44	-411.880
	Fe_tri K	3.800e-006 5.270e-005	3.800e-006 5.270e-005			Fe_tri	3.800e-006 Fe_tri(OH)2+	3.612e-006	2.640e-006	-5.442	-5.578
	Mg Min	9.719e-004 3.951e-007	9.719e-004 3.951e-007			-0.136	Fe_triOH+2	1.037e-007	2.958e-008	-6.984	-7.529
	Na. S	4.183e-004	4.183e-004			-0.545	Fe tri (OH) 3	8 344-008	9 163-008	-7 079	-7 038
		Description of	solution			0.041	Fe trign+	3 698-010	2 702-010	_9 /132	_9 568
		Jescription of	Solucion			-0.136	Po trita	2 9590 010	1 7006 011	9.402	10 769
		pH	= 5.434	Charge	e balance	-1.226	re_urs	2.0050-010	0.005 011	-9.944	-10.705
equilibrium		pe	= 15.108	ACJUS	ed to redux	-0.545	Fe_trici+2	2.8006-010	8.005e-011	-9.002	-10.097
	Activ	aty of water	_ // (001					- co- o44	E EEA 044	40 440	40.004
	Ic	nic strength	= 4.068e-0	01		-0.136	Fe_triCl2+	7.627e-011	5.574e-011	-10.118	-10.254
	Id Mass d Total alkal:	onic strength of water (kg) inity (eq/kg)	= 4.068e-0 = 1.000e+0 = 2.967e-0	01 00 02		-0.136 -0.136	Fe_triCl2+ Fe_tri(OH)4-	7.627e-011 3.081e-011	5.574e-011 2.252e-011	-10.118 -10.511	-10.254 -10.647
	I Mass ( Total alkal: Total Tempera	nic strength of water (kg) inity (eg/kg) CO2 (mol/kg) ature (deg C)	= 4.068e-0 = 1.000e+0 = 2.967e-0 = 1.389e-0 = 25.000	01 00 02 01		-0.136 -0.136 -0.136	Fe_triCl2+ Fe_tri (OH) 4- Fe_tri (SO4) 2-	7.627e-011 3.081e-011 1.173e-011	5.574e-011 2.252e-011 8.569e-012	-10.118 -10.511 -10.931	-10.254 -10.647 -11.067
Percent erro	Id Mass of Total alkal: Total Tempera Electrical or, 100*(Cat- An	nic strength f water (kg) inity (eg/kg) CO2 (mol/kg) ature (deg C) balance (eq) )/(Cat+[An])	$\begin{array}{rcl} & & 0.391 \\ = & 4.068e^{-0} \\ = & 1.000e^{+0} \\ = & 2.967e^{-0} \\ = & 1.389e^{-0} \\ = & 2.518e^{-0} \\ = & 0.00 \end{array}$	01 00 02 01 14		-0.136 -0.136 -0.136 -2.179	Fe_tri(12+ Fe_tri(0H)4- Fe_tri(504)2- Fe_tri2(0H)2+4	7.627e-011 3.081e-011 1.173e-011 3.556e-012	5.574e-011 2.252e-011 8.569e-012 2.355e-014	-10.118 -10.511 -10.931 -11.449	-10.254 -10.647 -11.067 -13.628
Percent erro	I Mass ( Total alkal: Total Total Total Electrical Cat- An (Cat- An	nic strength of water (kg) inity (eg/kg) CO2 (mol/kg) ature (deg C) balance (eg)  )/(Cat+ An ) Iterations Total H	$\begin{array}{rcl} & - & 0.391 \\ = & 4.068e-0 \\ = & 1.000e+0 \\ = & 2.967e-0 \\ = & 1.389e-0 \\ = & 25.000 \\ = & 25.518e-0 \\ = & 0.00 \\ = & 47 \\ = & 1.110421e \end{array}$	01 00 02 01 14 +002		-0.136 -0.136 -0.136 -2.179 0.041	Fe_tri(CH)4- Fe_tri(SO4)2- Fe_tri2(CH)2+4 Fe_tri23	7.627e-011 3.081e-011 1.173e-011 3.556e-012 7.912e-013	5.574e-011 2.252e-011 8.569e-012 2.355e-014 8.689e-013	-10.118 -10.511 -10.931 -11.449 -12.102	-10.254 -10.647 -11.067 -13.628 -12.061
Percent erro	I Mass o Total alkal Total Tenper Electrical or, 100*(Cat- An	nic strength of water (kg) (CO2 (mol/kg) ature (deg C) balance (eg) )/(Cat+[An]) Iterations Total H Total O	- 0.991 = 4.068e-0 = 1.000e+0 = 2.967e-0 = 1.389e-0 = 2.518e-0 = 0.00 = 47 = 1.110421e = 5.587723e	01 00 02 01 14 +002 +001		-0.136 -0.136 -0.136 -2.179 0.041 -3.405	Fe_triCl2+ Fe_tri(OH)4- Fe_tri(SO4)2- Fe_tri2(OH)2+4 Fe_triCl3 Fe_tri3(OH)4+5	7.627e-011 3.081e-011 1.173e-011 3.556e-012 7.912e-013 3.297e-014	5.574e-011 2.252e-011 8.569e-012 2.355e-014 8.689e-013 1.299e-017	-10.118 -10.511 -10.931 -11.449 -12.102 -13.482	-10.254 -10.647 -11.067 -13.628 -12.061 -16.886
Percent erro	II Mass ( Total alkal: Total Tamper Electrical or, 100* (Cat- An	nic strength of water (kg) (C2 (ml/kg) balance (eg) )/(Cat+[An]) Iterations Total H Total O Distribution o	- 0.991 = 4.068e-0 = 1.000e+0 = 2.967e-0 = 25.000 = 25.000 = 0.00 = 47 = 1.110421e = 5.587723e f species	01 00 02 01 14 +002 +001		-0.136 -0.136 -2.179 0.041 -3.405	Fe_triCl2+ Fe_tri (CH)4- Fe_tri (SO4)2- Fe_tri2 (CH)2+4 Fe_triCl3 Fe_tri3 (CH)4+5 Fe_triBO4+2	7.627e-011 3.081e-011 1.173e-011 3.556e-012 7.912e-013 3.297e-014 9.330e-015	5.574e-011 2.252e-011 8.569e-012 2.355e-014 8.689e-013 1.299e-017 2.662e-015	-10.118 -10.511 -10.931 -11.449 -12.102 -13.482 -14.030	-10.254 -10.647 -11.067 -13.628 -12.061 -16.886 -14.575
Percent erro	II Mass ( Total alkal: Total Tanper Electrical or, 100* (Cat- An	mic strength of water (kg) mity (eq/kg) CO2 (mol/kg) ature (deg C) balance (eg)  )/(Cat+[An]) Iterations Total H Total 0 Distribution o	- 0.991 = 4.068e-0 = 1.000e+0 = 2.967e-0 = 1.389e-0 = 25.000 = 2.518e-0 = 0.00 = 47 = 1.110421e = 5.587723e	01 00 02 01 14 ++002 ++001		-0.136 -0.136 -2.179 0.041 -3.405 -0.545 H(0)	Fe_tri(12+ Fe_tri(0H)4- Fe_tri(0A)2- Fe_tri2(0H)2+4 Fe_triCl3 Fe_tri3(0H)4+5 Fe_triHSO4+2 0,000e+000	7.627e-011 3.081e-011 1.173e-011 3.556e-012 7.912e-013 3.297e-014 9.330e-015	5.574e-011 2.252e-011 8.569e-012 2.355e-014 8.689e-013 1.299e-017 2.662e-015	-10.118 -10.511 -10.931 -11.449 -12.102 -13.482 -14.030	-10.254 -10.647 -11.067 -13.628 -12.061 -16.886 -14.575
Percent erro	I NASS ( Mass ( Total alkal) Total Tempera Electrical or, 100*(Cat- An	nic strength fr water (kg) CO2 (mol/kg) Atree (deg C) balance (eg) )/(Cat+ An] Iterations Total H Total O Distribution o	- 0.991 = 4.068e-0 = 1.000e+0 = 2.967e-0 = 2.518e-0 = 2.518e-0 = 0.00 = 47 = 1.110421e = 5.587723e f species	01 00 02 01 14 ++002 ++001 	Log	-0.136 -0.136 -2.179 0.041 -3.405 -0.545 H(0) 0.041	Fe_tri(12+ Fe_tri(0H)4- Fe_tri(SO4)2- Fe_tri2(0H)2+4 Fe_triC13 Fe_triG13 Fe_triH5O4+2 0.000e+000 H2 E_770-005	7.627e-011 3.081e-011 1.173e-011 3.556e-012 7.912e-013 3.297e-014 9.330e-015 0.000e+000	5.574e-011 2.252e-011 8.569e-012 2.355e-014 8.689e-013 1.299e-017 2.662e-015 0.000e+000	-10.118 -10.511 -10.931 -11.449 -12.102 -13.482 -14.030 -44.396	-10.254 -10.647 -11.067 -13.628 -12.061 -16.886 -14.575 -44.355
Percent erro	I Mas Mass Total alkali Total Total Impea Electrical or, 100*(Cat- An Jock Cat- An Species	nic strength fr water (kg) CO2 (mol/kg) Atnre (deg C) halarce (eg) )/(Cat+ An]) Iterations Total H Total O Distribution o Molality	- 0.391 = 4.068e-0 = 1.000e+0 = 2.967e-0 = 2.967e-0 = 25.000 = 0.00 = 0.00 = 47 = 1.110421e = 5.587723e f species	01 00 02 01 14 +002 +001 Log Molality	Log Activity	-0.136 -0.136 -2.179 0.041 -3.405 -0.545 H(0) 0.041 K	Fe_tri(12+ Fe_tri(0t)4- Fe_tri(304)2- Fe_tri2(0t)2+4 Fe_triC13 Fe_tri3(0t)4+5 Fe_triH504+2 0.000e+000 H2 5.270e=005 K+	7.627e-011 3.081e-011 1.173e-011 3.556e-012 7.912e-013 3.297e-014 9.330e-015 0.000e+000 5.222e-005	5.574e-011 2.252e-011 8.569e-012 2.355e-014 8.689e-013 1.299e-017 2.662e-015 0.000e+000 3.439e-005	-10.118 -10.511 -10.931 -11.449 -12.102 -13.482 -14.030 -44.396 -4.282	-10.254 -10.647 -11.067 -13.628 -12.061 -16.886 -14.575 -44.355 -44.464
Percent erro	I Mas Mass Total alkali Total Ital Impea Electrical or, 100*(Cat- An geccies	nic strength f water (kg) finity (eg/kg) CO2 (mol/kg) Dolaroe (eg) J)/(Cat+ An]) Iterations Total M Distribution o Molality 4.767e-006	- 0.391 = 4.068e-0 = 1.000e+0 2.967e-0 = 2.567e-0 = 2.518e-0 = 0.00 = 47 = 1.110421e = 5.587723e f species Activity 3.678e-006	01 00 02 01 14 +002 +001 Log Molality -5.322	Log Activity -5.434	-0.136 -0.136 -2.179 0.041 -3.405 -0.545 H(0) 0.041 K -0.181	Fe_tri(12+ Fe_tri(0t)4- Fe_tri(304)2- Fe_tri2(0t)2+4 Fe_triC13 Fe_tri3(0t)4+5 Fe_triHE04+2 0.000e+000 H2 5.270e-005 K+ KS04-	7.627e-011 3.081e-011 1.173e-011 3.556e-012 7.912e-013 3.297e-014 9.330e-015 0.000e+000 5.222e-005 4.793e-007	5.574e-011 2.252e-011 8.569e-012 2.355e-014 8.689e-013 1.299e-017 2.662e-015 0.000e+000 3.439e-005 3.503e-007	-10.118 -10.511 -10.931 -11.449 -12.102 -13.482 -14.030 -44.396 -4.282 -6.319	-10.254 -10.647 -11.067 -13.628 -12.061 -16.886 -14.575 -44.355 -44.454 -6.456
Percent error	I Mas Mass Total alkali Total Ital Impac Electrical or, 100*(Cat- An gaecies H+ CH-	nic strength f water (kg) inity (eg/kg) CO2 (mol/kg) Dolaroe (eg) J/ (Cat+ An]) Iterations Total M Distribution o Distribution o Molality 4.767e-006 4.154e-009	<ul> <li>- 0.331</li> <li>- 4.068e-0</li> <li>= 1.000e+0</li> <li>2.967e-0</li> <li>= 1.389e-0</li> <li>0.00</li> <li>= 4.7</li> <li>= 1.110421e</li> <li>= 5.587723e</li> <li>f species</li> <li>Activity</li> <li>3.678e-006</li> <li>2.698e-009</li> </ul>	01 00 02 01 14 +002 +001 Log Molality -5.322 -8.382	Log Activity -5.434 -8.569	-0.136 -0.136 -2.179 0.041 -3.405 -0.545 H(0) 0.041 K -0.181 -0.136	Fe_tri(12+ Fe_tri(0t)4- Fe_tri(304)2- Fe_tri2(0t)2+4 Fe_triC13 Fe_tri3(0t)4+5 Fe_triHE04+2 0.000e+000 H2 5.270e-005 K+ KS04- KCH	7.627e-011 3.081e-011 1.173e-011 3.556e-012 7.912e-013 3.297e-014 9.330e-015 0.000e+000 5.222e-005 4.793e-007 2.926e-014	5.574e-011 2.252e-011 8.569e-012 2.355e-014 8.689e-013 1.299e-017 2.662e-015 0.000e+000 3.439e-005 3.503e-007 3.214e-014	-10.118 -10.511 -10.931 -11.449 -12.102 -13.482 -14.030 -44.396 -4.282 -6.319 -13.534	-10.254 -10.647 -11.067 -13.628 -12.061 -16.886 -14.575 -44.355 -4.464 -6.456 -13.493
Percent error  Log Gemma -0.113 -0.187	I Mass Mass Total alkali Total Total Total Total Species H+ CH- H2O	nic strength f water (kg) inity (eg/kg) CO2 (mol/kg) CO2 (mol/kg) Dalance (eg) J)/(Cat+ An ) Iterations Total H Total O Distribution o Molality 4.767e-006 4.154e-009 5.551e+001	- 0.33 = 4.069-0 = 1.000+0 = 2.967-0 = 2.967-0 = 2.507 = 25.000 = 2.518e-0 = 0.00 = 47 Activity 3.678e-006 2.698e-009 9.911e-001	01 00 02 01 14 +002 +001 Log Molality -5.322 -8.382 1.744	Log Activity -5.434 -8.569 -0.004	-0.136 -0.136 -2.179 0.041 -3.405 -0.545 H(0) 0.041 K -0.181 -0.136 0.041 My	Fe_tri(12+ Fe_tri(0t)4- Fe_tri(304)2- Fe_tri2(0t)2+4 Fe_triC13 Fe_tri3(0t)4+5 Fe_triHE04+2 0.000e+000 H2 5.270e-005 K+ KS04- KCH 9.719e-004	7.627e-011 3.081e-011 1.173e-011 3.556e-012 7.912e-013 3.297e-014 9.330e-015 0.000e+000 5.222e-005 4.793e-007 2.926e-014	5.574e-011 2.252e-011 8.569e-012 2.355e-014 8.689e-013 1.299e-017 2.662e-015 0.000e+000 3.439e-005 3.503e-007 3.214e-014	-10.118 -10.511 -10.931 -11.449 -12.102 -13.482 -14.030 -44.396 -4.282 -6.319 -13.534	-10.254 -10.647 -11.067 -13.628 -12.061 -16.886 -14.575 -44.355 -44.355 -4.464 -6.456 -13.493
Percent error  Log Gamma -0.113 -0.187 0.000 C(-4)	I Mass Mass Total alkali Total Total Total Total Electrical Electrical Cat.  An Species H+ CH- H2O 0.000e+000	nic strength f water (kg) inity (eg/kg) CO2 (mol/kg) CO2 (mol/kg) Dalance (eg) J)/(Cat+ An ) Iterations Total H Total O Distribution o Molality 4.767e-006 4.154e-009 5.551e+001	- 0.33 - 0.362-0 = 1.000+0 = 2.967-0 = 2.967-0 = 2.507 = 25.000 = 25.000 = 25.000 = 0.00 = 47 Activity 3.678e-006 2.698e-009 9.911e-001	01 00 02 01 14 +002 +001 Log Molality -5.322 -8.382 1.744	Log Activity -5.434 -8.569 -0.004	-0.136 -0.136 -2.179 0.041 -3.405 -0.545 H(0) 0.041 K -0.181 -0.136 0.041 My	Fe_tri(12+ Fe_tri(0t)4- Fe_tri(304)2- Fe_tri2(0t)2+4 Fe_tri2(0t)4+5 Fe_triHED4+2 0.000e+000 H2 5.270e-005 K+ KS04- KCH 9.719e-004 Mg+2	7.627e-011 3.081e-011 1.173e-011 3.556e-012 7.912e-013 3.297e-014 9.330e-015 0.000e+000 5.222e-005 4.793e-007 2.926e-014 8.364e-004	5.574e-011 2.252e-011 8.569e-012 2.355e-014 8.689e-013 1.299e-017 2.662e-015 0.000e+000 3.439e-005 3.503e-007 3.214e-014 2.511e-004	-10.118 -10.511 -10.931 -11.449 -12.102 -13.482 -14.030 -44.396 -4.282 -6.319 -13.534 -3.078	-10.254 -10.647 -11.067 -13.628 -12.061 -16.886 -14.575 -44.355 -44.355 -4.464 -6.456 -13.493 -3.600
Percent error  Log Gamma -0.113 -0.187 0.000 C(-4) 0.041	I Mass Mass Total aldai Total Total Total Total Total Species H+ CH- H2O CH- H2O CH4	nic strength f water (kg) inity (eg/kg) CO2 (mol/kg) CO2 (mol/kg) Dislance (eg) J)/(Cat+ An ) Iterations Total H Total O Distribution o Distribution o A.167e-006 4.154e-009 5.551e+001 0.000e+000	- 0.33 - 0.362-0 = 1.000+0 = 2.967-0 = 2.967-0 = 2.507 = 25.000 = 25.000 = 25.000 = 0.00 = 47 Activity 3.678e-006 2.698e-009 9.911e-001 0.000e+000	01 00 02 11 14 +002 +001 Molality -5.322 -8.382 1.744 -141.384	Log Activity -5.434 -8.569 -0.004 -141.344	-0.136 -0.136 -2.179 0.041 -3.405 -0.545 H(0) 0.041 K -0.181 -0.136 0.041 Mg -0.523 0.041	Fe_tri(12+ Fe_tri(0t)4- Fe_tri(304)2- Fe_tri2(0t)2+4 Fe_tri2(0t)4+5 Fe_triHE04+2 0.000e+000 H2 5.270e-005 K+ KS04- KCH 9.719e-004 Mg+2 Mg504	7.627e-011 3.081e-011 1.173e-011 3.556e-012 7.912e-013 3.297e-014 9.330e-015 0.000e+000 5.222e-005 4.793e-007 2.926e-014 8.364e-004 7.770e-005	5.574e-011 2.252e-011 8.569e-012 2.355e-014 8.689e-013 1.299e-017 2.662e-015 3.000e+000 3.439e-005 3.503e-007 3.214e-014 2.511e-004 8.533e-005	-10.118 -10.511 -10.931 -11.449 -12.102 -13.482 -14.030 -44.396 -4.282 -6.319 -13.534 -3.078 -4.110	-10.254 -10.647 -11.067 -13.628 -12.061 -16.886 -14.575 -44.355 -44.355 -4.464 -6.456 -13.493 -3.600 -4.069
Percent error  Log Gamma -0.113 -0.187 0.000 C(-4) 0.041 C(4)	II Mass Total alkali Tital Tital Tital Tital Tital Tital Species H+ CH- H2O CH- H2O CH- H2O CH- H2O CH- M2O CH- CH- CH- CH- CH- CH- CH- CH- CH- CH-	nic strength f water (kg) inity (eg/kg) CO2 (mol/kg) CO2 (mol/kg) Dislance (eg) J)/(Cat+ An ) Iterations Total H Total O Distribution o Nolality 4.767e-006 4.154e-009 5.551e+001 0.000e+000	- 0.39 - 0.39 - 0.00e+0 - 1.000e+0 - 2.967e-0 - 2.387e-0 - 2.500 - 2.500 - 2.500 - 0.00 - 47 - 0.10421e - 5.587723e f species Activity 3.678e-006 2.698e-009 9.911e-001 0.000e+000 1.200e.001	01 00 02 11 14 +002 +001 	Log Activity -5.434 -8.569 -0.004 -141.344	-0.136 -0.136 -2.179 0.041 -3.405 -0.545 H(0) 0.041 K -0.181 -0.136 0.041 My -0.523 0.041 0.136	Fe_tri(12+ Fe_tri(0t)4- Fe_tri(304)2- Fe_tri2(0t)2+4 Fe_tri2(0t)4+5 Fe_triHSD4+2 0.000e+000 H2 5.270e-005 K+ KSO4- KCH 9.719e-004 Mg+2 Mg5O4 MgHO3+	7.627e-011 3.081e-011 1.173e-011 3.556e-012 7.912e-013 3.297e-014 9.330e-015 0.000e+000 5.222e-005 4.793e-007 2.926e-014 8.364e-004 7.770e-005 5.780e-005	5.574e-011 2.252e-011 8.569e-012 2.355e-014 8.689e-013 1.299e-017 2.662e-015 3.602e-015 3.503e-007 3.214e-014 2.511e-004 8.533e-005 4.225e-005	-10.118 -10.511 -10.931 -11.449 -12.102 -13.482 -14.030 -44.396 -4.282 -6.319 -13.534 -3.078 -4.110 -4.238	-10.254 -10.647 -11.067 -13.628 -12.061 -16.886 -14.575 -44.355 -44.355 -4.464 -6.456 -13.493 -3.600 -4.069 -4.374
Percent error  Log Gamma -0.113 -0.187 0.000 C(-4) 0.041 0.041	II Mass Total alkali Tital Tital Tital Tital Tital Spacies H+ CH- H2O CH- H2O CH- H2O CH- 1.389e-001 C22	mic strength f water (kg) inity (eg/kg) CO2 (mol/kg) CO2 (mol/kg) CO2 (mol/kg) Distribution (kg C) balance (eg) J)/(Cat+ An ) Iterations Total O Distribution o Distribution o Distribution o 4.154e-009 5.551e+001 0.000e+000 1.092e-001	- 0.39 - 0.39 - 0.00e+0 - 1.000e+0 - 2.967e-0 - 2.397e-0 - 2.507 - 2.508-0 - 0.00 - 47 - 0.10421e - 5.587723e f species Activity 3.678e-006 2.698e-009 9.911e-001 0.000e+000 1.200e-001 1.400e-001	01 00 02 11 14 +002 +001 Molality -5.322 -8.382 1.744 -141.384 -0.962	Log Activity -5.434 -8.569 -0.004 -141.344 -0.921	$\begin{array}{c} -0.136\\ -0.136\\ -2.179\\ 0.041\\ -3.405\\ -0.545\\ +0.0545\\ +0.0181\\ -0.181\\ -0.136\\ 0.041\\ My\\ -0.523\\ 0.041\\ -0.523\\ 0.041\\ -0.136\\ 0.041\\ -0.136\\ 0.041\\ \end{array}$	Fe_tri(12+ Fe_tri(0t)4- Fe_tri(304)2- Fe_tri2(0t)2+4 Fe_tri3(0t)4+5 Fe_triHS04+2 0.000e+000 H2 5.270e-005 K+ KS04- KCH 9.719e-004 Mg+2 Mg504 Mg403+	7.627e-011 3.081e-011 1.173e-011 3.556e-012 7.912e-013 3.297e-014 9.330e-015 0.000e+000 5.222e-005 4.793e-007 2.926e-014 8.364e-004 7.770e-005 5.780e-005 4.000e-008	5.574e-011 2.252e-011 8.569e-012 2.355e-014 8.689e-013 1.299e-017 2.662e-015 3.602e-015 3.503e-007 3.214e-014 2.511e-004 8.533e-005 4.225e-005 4.393e-08	-10.118 -10.511 -10.931 -11.449 -12.102 -13.482 -14.030 -44.396 -4.282 -6.319 -13.534 -3.078 -4.110 -4.238 -7.398	-10.254 -10.647 -11.067 -13.628 -12.061 -16.886 -14.575 -44.355 -44.355 -4.464 -6.456 -13.493 -3.600 -4.069 -4.374 -7.357
Percent error  Log Gamma -0.113 -0.187 0.000 C(-4) 0.041 -0.152	II Mass Total alkali Tital Tital Tital Tital Tital Tital Tital Spacies H+ CH- H2O CH- H2O CH- H2O CH- H2O CH- H2O CH- H2O CH- H2O CH- CH- H2O CH- CH- H2O CH- CH- CH- H2O CH- CH- H2O CH- CH- CH- CH- CH- CH- CH- CH- CH- CH-	mic strength f water (kg) inity (eq/kg) CO2 (mol/kg) CO2 (mol/kg) CO2 (mol/kg) Distribution (kg C) balance (eq) J)/(Cat+ An ) Iterations Total O Distribution o Distribution o Distribution o 4.154e-009 5.551e+001 0.000e+000 1.092e-001 2.042e-002	- 0.39 - 0.39 - 0.00e+0 - 1.000e+0 - 2.967e-0 - 2.397e-0 - 2.507 - 2.508-0 - 0.00 - 47 - 0.10421e - 5.587723e f species Activity 3.678e-006 2.698e-009 9.911e-001 0.000e+000 1.200e-001 1.438e-002	01 00 02 01 14 +002 +001 Molality -5.322 -8.382 1.744 -141.384 -0.962 0.0962 0.000	Log Activity -5.434 -8.569 -0.004 -141.344 -0.921 -1.842 2.452	$\begin{array}{c} -0.136\\ -0.136\\ -2.179\\ 0.041\\ -3.405\\ -0.545\\ +0.0545\\ +0.0181\\ -0.181\\ -0.136\\ 0.041\\ My\\ -0.523\\ 0.041\\ -0.523\\ 0.041\\ -0.136\\ 0.041\\ -0.136\\ 0.041\\ \end{array}$	Fe_tri(12+ Fe_tri(0t)4- Fe_tri(304)2- Fe_tri2(0t)2+4 Fe_tri3(0t)4+5 Fe_triHS04+2 0.000e+000 H2 5.270e-005 K+ KS04- KCH 9.719e-004 Mg+2 Mg504 Mg403+ Mg003 Mg0H+	7.627e-011 3.081e-011 1.173e-011 3.556e-012 7.912e-013 3.297e-014 9.330e-015 0.000e+000 5.222e-005 4.793e-007 2.926e-014 8.364e-004 7.770e-005 5.780e-005 4.000e-008 3.362e-010	5.574e-011 2.252e-011 8.569e-012 2.355e-014 8.689e-013 1.299e-017 2.662e-015 3.602e-015 3.503e-007 3.214e-014 2.511e-004 8.533e-005 4.225e-005 4.239a-008 2.457e-010	-10.118 -10.511 -10.931 -11.449 -12.102 -13.482 -14.030 -44.396 -4.282 -6.319 -13.534 -3.078 -4.110 -4.238 -7.398 -9.473	-10.254 -10.647 -11.067 -13.628 -12.061 -16.886 -14.575 -44.355 -44.355 -4.464 -6.456 -13.493 -3.600 -4.069 -4.374 -7.357 -9.610
Percent error  Log Gamma -0.113 -0.187 0.000 C(-4) 0.041 -0.152 -0.152	II Mass Total alkali Tital Tital Tital Tital Tital Tital Tital Spacies H+ CH- H2O CH- H2O CH- H2O CH- H2O CH- CH- CH- CH- CH- CH- CH- CH- CH- CH-	mic strength f water (kg) inity (eq/kg) CO2 (mol/kg) CO2 (mol/kg) CO2 (mol/kg) Distribution (kg C) Falance (eq) J)/(Cat+ An ) Iterations Total H Total O Distribution o Distribution o Distribution o 0.001 4.154e-009 5.551e+001 0.000e+000 1.092e-001 2.042e-002 9.115e-003	- 0.33 - 0.36 - 0.000+0 - 1.000+0 - 2.967-0 - 2.367-0 - 2.507 - 2.500 - 2.500 - 2.500 - 2.500 - 0.00 - 47 - 0.00 - 0.00 - 47 - 0.00 - 47 - 0.00 - 47 - 0.00 - 0.00 - 47 - 0.00 - 0.00 - 47 - 0.00 - 0	01 00 02 11 14 +002 +001 Molality -5.322 -8.382 1.744 -141.384 -0.962 -1.690 -2.040	Log Activity -5.434 -8.569 -0.004 -141.344 -0.921 -1.842 -2.193	$\begin{array}{c} -0.136\\ -0.136\\ -2.179\\ 0.041\\ -3.405\\ -0.545\\ H(0)\\ 0.041\\ K\\ -0.181\\ -0.136\\ 0.041\\ My\\ -0.523\\ 0.041\\ My\\ -0.523\\ 0.041\\ -0.136\\ 0.041\\ -0.012\\ -0.02\\ 0.02\\ -0.02$	Fe_tri(12+ Fe_tri(0t)4- Fe_tri(304)2- Fe_tri2(0t)2+4 Fe_tri3(0t)4+5 Fe_triHS04+2 0.000e+000 H2 5.270e-005 K+ KS04- KCH 9.719e-004 Mg+2 Mg504 Mg503 MgCH+ 3.951e-007	7.627e-011 3.081e-011 1.173e-011 3.556e-012 7.912e-013 3.297e-014 9.330e-015 0.000e+000 5.222e-005 4.793e-007 2.926e-014 8.364e-004 7.770e-005 5.780e-005 4.000e-008 3.362e-010	5.574e-011 2.252e-011 8.569e-012 2.355e-014 8.689e-013 1.299e-017 2.662e-015 3.602e-015 3.503e-007 3.214e-014 2.511e-004 8.533e-005 4.225e-005 4.393e-008 2.457e-010	-10.118 -10.511 -10.931 -11.449 -12.102 -13.482 -14.030 -44.396 -4.282 -6.319 -13.534 -3.078 -4.110 -4.238 -7.398 -9.473	-10.254 -10.647 -11.067 -13.628 -12.061 -16.886 -14.575 -44.355 -44.355 -4.464 -6.456 -13.493 -3.600 -4.069 -4.374 -7.357 -9.610
Percent error  Log Gamma -0.113 -0.187 0.000 C(-4) 0.041 C(4) 0.041 -0.152 -0.152 -0.136	II Mass Total alkali Tital Tital Tital Tital Tital Tital Tital Tital Species H+ CH- H2O 0.000e+000 CH4 1.389e-001 CC2 HC03- CaHC03+ MgHC03+	mic strength f water (kg) inity (eq/kg) CO2 (mol/kg) CO2	- 0.39 - 0.39 - 0.00e+0 - 1.000e+0 - 2.967e-0 - 2.387e-0 - 2.507 - 2.508 - 0.00 - 47 - 0.10 - 47 - 0.10 - 47 - 0.10 - 47 - 0.00 - 0	01 00 02 11 14 +002 +001 Molality -5.322 -8.382 1.744 -141.384 -0.962 -1.690 -2.040 -4.238	Log Activity -5.434 -8.569 -0.004 -141.344 -0.921 -1.842 -2.193 -4.374	$\begin{array}{c} -0.136\\ -0.136\\ -0.136\\ -2.179\\ 0.041\\ -3.405\\ -0.545\\ H(0)\\ 0.041\\ K\\ -0.181\\ -0.136\\ 0.041\\ My\\ -0.523\\ 0.041\\ -0.136\\ 0.041\\ -0.136\\ 0.041\\ -0.136\\ 0.041\\ -0.136\\ 0.041\\ -0.136\\ Mn(2)\\ -0.576\end{array}$	Fe_tri(12+ Fe_tri(12+ Fe_tri(304)2- Fe_tri2(0+)2+4 Fe_tri2(0+)2+4 Fe_tri3(0+)4+5 Fe_triHSD4+2 0.000e+000 H2 5.270e-005 K+ KSO4- KCH 9.719e-004 Mg+2 MgSO4 MgHO3+ MgCO3 MgCH+ 3.951e-007 Mn+2	7.627e-011 3.081e-011 1.173e-011 3.556e-012 7.912e-013 3.297e-014 9.330e-015 0.000e+000 5.222e-005 4.793e-007 2.926e-014 8.364e-004 7.770e-005 5.780e-005 4.000e-008 3.362e-010 2.2228e-007	5.574e-011 2.252e-011 8.569e-012 2.355e-014 8.689e-013 1.299e-017 2.662e-015 3.602e-015 3.503e-007 3.214e-014 2.511e-004 8.533e-005 4.225e-005 4.239a-008 2.457e-010 5.917e-008	-10.118 -10.511 -10.931 -11.449 -12.102 -13.482 -14.030 -44.396 -4.282 -6.319 -13.534 -3.078 -4.110 -4.238 -7.398 -9.473 -6.652	-10.254 -10.647 -11.067 -13.628 -12.061 -16.886 -14.575 -44.355 -44.355 -4.464 -6.456 -13.493 -3.600 -4.069 -4.374 -7.357 -9.610 -7.228
Percent error 	II MES Total alkal. Total Total Total Total Total Total Total Species H* CH- H2O CH- CH- H2O CH- H2O CH- H2O CH- H2O CH- CH- H2O CH- CH- H2O CH- CH- H2O CH- CH- H2O CH- CH- H2O CH- CH- H2O CH- CH- H2O CH- CH- H2O CH- CH- H2O CH- CH- H2O CH- CH- H2O CH- CH- CH- CH- CH- CH- CH- CH- CH- CH-	mic strength f water (kg) inity (eq/kg) CO2 (mol/kg) CO2	- 0.39 - 0.39 - 0.00e+0 - 1.000e+0 - 2.967e-0 - 2.967e-0 - 2.507e-0 - 0.00 - 2.508 - 0.00 - 47 -	01 00 02 11 14 +002 +001 Molality -5.322 -8.382 1.744 -141.384 -0.962 -1.690 -2.040 -4.238 -4.288	Log Activity -5.434 -8.569 -0.004 -141.344 -0.921 -1.842 -2.193 -4.374 -4.424	$\begin{array}{c} -0.136\\ -0.136\\ -0.136\\ -2.179\\ 0.041\\ -3.405\\ -0.545\\ H(0)\\ 0.041\\ K\\ -0.181\\ -0.136\\ 0.041\\ My\\ -0.523\\ 0.041\\ -0.136\\ 0.041\\ -0.136\\ 0.041\\ -0.136\\ Mn(2)\\ -0.576\\ -0.136\end{array}$	Fe_tri(12+ Fe_tri(12+ Fe_tri(304)2- Fe_tri2(0+)2+4 Fe_tri2(0+)2+4 Fe_tri3(0+)4+5 Fe_triHED4+2 0.000e+000 H2 5.270e-005 K+ KSO4- KCH 9.719e-004 Mg+2 MgSO4 MgHO3+ MgC03 MgCH+ 3.951e-007 Mn+2 MHCO3+	7.627e-011 3.081e-011 1.173e-011 3.556e-012 7.912e-013 3.297e-014 9.330e-015 0.000e+000 5.222e-005 4.793e-007 2.926e-014 8.364e-004 7.770e-005 5.780e-005 4.000e-008 3.362e-010 2.228e-007 1.037e-007	5.574e-011 2.252e-011 8.569e-012 2.355e-014 8.689e-013 1.299e-017 2.662e-015 3.602e-015 3.503e-007 3.214e-014 2.511e-004 8.533e-005 4.225e-005 4.239a-008 2.457e-010 5.917e-008 7.581e-008	-10.118 -10.511 -10.931 -11.449 -12.102 -13.482 -14.030 -44.396 -4.282 -6.319 -13.534 -3.078 -4.110 -4.238 -7.398 -9.473 -6.652 -6.984	-10.254 -10.647 -11.067 -13.628 -12.061 -16.886 -14.575 -44.355 -44.355 -4.464 -6.456 -13.493 -3.600 -4.069 -4.374 -7.357 -9.610 -7.228 -7.120
Percent error 	II MESS Total alkal. Total Total Total Total Total Total Total Species H* CH- H2O CH- CH- H2O CH- H2O CH- H2O CH- CH- H2O CH- CH- H2O CH- CH- H2O CH- H2O CH- H2O CH- CH- H2O CH- CH- CH- CH- CH- CH- CH- CH- CH- CH-	mic strength f water (kg) inity (eq/kg) CO2 (mol/kg) CO2	- 0.39 - 0.39 - 0.000+0 - 1.000+0 - 2.957-0 - 2.957-0 - 2.507 - 2.507 - 2.508-0 - 0.00 - 47 - 47	01 00 02 11 14 +002 +001 Molality -5.322 -8.382 1.744 -141.384 -0.962 -1.690 -2.040 -4.238 -4.288 -5.008	Log Activity -5.434 -8.569 -0.004 -141.344 -0.921 -1.842 -2.193 -4.374 -4.424 -4.968	$\begin{array}{c} -0.136\\ -0.136\\ -0.136\\ -2.179\\ 0.041\\ -3.405\\ -0.545\\ H(0)\\ 0.041\\ K\\ -0.181\\ -0.136\\ 0.041\\ My\\ -0.523\\ 0.041\\ -0.136\\ 0.041\\ -0.136\\ 0.041\\ -0.136\\ 0.041\\ -0.136\\ Mn(2)\\ -0.576\\ -0.136\\ -0.136\\ -0.136\\ -0.136\end{array}$	Fe_tri(12+ Fe_tri(12+ Fe_tri(304)2- Fe_tri2(0+)2+4 Fe_tri2(0+)2+4 Fe_tri3(0+)4+5 Fe_triHSD4+2 0.000e+000 H2 5.270e-005 K+ KSO4- KCH 9.719e-004 Mg+2 Mg5O4 Mg+03+ MgC03+ MgC03+ MgC03+ Mg+C03+ Mg+C1+	7.627e-011 3.081e-011 1.173e-011 3.556e-012 7.912e-013 3.297e-014 9.330e-015 0.000e+000 5.222e-005 4.793e-007 2.926e-014 8.364e-004 7.770e-005 5.780e-005 4.000e-008 3.362e-010 2.228e-007 1.037e-007 5.141e-008	5.574e-011 2.252e-011 8.569e-012 2.355e-014 8.689e-013 1.299e-017 2.662e-015 3.503e-007 3.214e-014 2.511e-004 8.533e-005 4.225e-005 4.239a-008 2.457e-010 5.917e-008 7.581e-008 3.757e-008	-10.118 -10.511 -10.931 -11.449 -12.102 -13.482 -14.030 -44.396 -4.282 -6.319 -13.534 -3.078 -4.110 -4.238 -7.398 -9.473 -6.652 -6.984 -7.289	-10.254 -10.647 -11.067 -13.628 -12.061 -16.886 -14.575 -44.355 -44.355 -4.464 -6.456 -13.493 -3.600 -4.069 -4.374 -7.357 -9.610 -7.228 -7.120 -7.425
Percent error 	II MBSS Total alkali Total Total Total Total Total Total Total Species H* CH- H2O CH- CH- H2O CH- H2O CH- CH- H2O CH- CH- H2O CH- CH- H2O CH- CH- H2O CH- CH- H2O CH- CH- H2O CH- CH- CH- CH- CH- CH- CH- CH- CD- CO CD- CH- CH- CD- CD- CD- CH- CD- CD- CD- CD- CD- CD- CD- CD- CD- CD	mic strength f water (kg) inity (eq/kg) CO2 (mol/kg) CO2	- 0.39 - 0.39 - 0.000+0 - 1.000+0 - 2.967-0 - 2.967-0 - 2.507 - 2.508-0 - 0.00 - 47 - 47 - 47 - 455-00 - 5.587723e f species Activity 3.678e-006 2.698e-009 9.911e-001 0.000e+000 1.200e-001 1.438e-002 6.417e-003 3.763e-005 1.077e-005 2.385e-006	01 00 02 11 14 +002 +001 Molality -5.322 -8.382 1.744 -141.384 -0.962 -1.690 -2.040 -4.238 -4.288 -5.008 -5.663	Log Activity -5.434 -8.569 -0.004 -141.344 -0.921 -1.842 -2.193 -4.374 -4.424 -4.968 -5.622	$\begin{array}{c} -0.136\\ -0.136\\ -0.136\\ -2.179\\ 0.041\\ -3.405\\ -0.545\\ H(0)\\ 0.041\\ K\\ -0.181\\ -0.136\\ 0.041\\ My\\ -0.523\\ 0.041\\ -0.136\\ 0.041\\ -0.136\\ 0.041\\ -0.136\\ $	Fe_tri(12+ Fe_tri(12+ Fe_tri(304)2- Fe_tri2(0+)2+4 Fe_tri3(0+)4+5 Fe_triHSD4+2 0.000e+000 H2 5.270e-005 K+ KSO4- KCH 9.719e-004 Mg+2 Mg5O4 Mg+03+ MgCO	7.627e-011 3.081e-011 1.173e-011 3.556e-012 7.912e-013 3.297e-014 9.330e-015 0.000e+000 5.222e-005 4.793e-007 2.926e-014 8.364e-004 7.770e-005 5.780e-005 4.000e-008 3.362e-010 2.228e-007 1.037e-007 5.141e-008 1.389e-008	5.574e-011 2.252e-011 8.569e-012 2.355e-014 8.689e-013 1.299e-017 2.662e-015 3.503e-007 3.214e-014 2.511e-004 8.533e-005 4.225e-005 4.239a-008 2.457e-010 5.917e-008 7.581e-008 3.757e-008 1.525e-008	-10.118 -10.511 -10.931 -11.449 -12.102 -13.482 -14.030 -44.396 -4.282 -6.319 -13.534 -3.078 -4.110 -4.238 -7.398 -9.473 -6.652 -6.984 -7.289 -7.857	-10.254 -10.647 -11.067 -13.628 -12.061 -16.886 -14.575 -44.355 -44.355 -4.464 -6.456 -13.493 -3.600 -4.069 -4.374 -7.357 -9.610 -7.228 -7.120 -7.425 -7.817
Percent error 	II MESS Total alkali Temper Total Terper Electrical ar, 100* (Cat- An Species H+ CH- H20 0.0000+000 CH 1.339e-001 CC2 CAHCO3+ MgHCO3+ Fe_diHCO3+ CaCO3 NaHCO3 CO3-2	mic strength f water (kg) imity (eq/kg) CO2 (mol/kg) CO2	- 0.39 - 0.39 - 0.000-0 - 1.000-0 - 2.967-0 - 2.967-0 - 2.507 - 2.500 - 2.500	01 00 02 11 14 +002 +001 Molality -5.322 -8.382 1.744 -141.384 -0.962 -1.690 -2.040 -4.238 -4.288 -5.068 -5.663 -6.127	Log Activity -5.434 -8.569 -0.004 -141.344 -0.921 -1.842 -2.193 -4.374 -4.424 -4.968 -5.622 -6.737	$\begin{array}{c} -0.136\\ -0.136\\ -0.136\\ -2.179\\ 0.041\\ -3.405\\ -0.545\\ H(0)\\ 0.041\\ K\\ -0.181\\ -0.136\\ 0.041\\ My\\ -0.523\\ 0.041\\ -0.136\\ 0.041\\ -0.136\\ 0.041\\ -0.136\\ -0.136\\ -0.136\\ -0.136\\ -0.136\\ -0.136\\ -0.136\\ -0.136\\ 0.041$	Fe_tri(12+ Fe_tri(12+ Fe_tri(304)2- Fe_tri2(0+)2+4 Fe_tri3(0+)4+5 Fe_triHS04+2 0.000e+000 H2 5.270e-005 K+ KS04- KCH 9.719e-004 Mg+20 Mg504 Mg504 Mg503 Mg603+ Mg703+ Mg70+	7.627e-011 3.081e-011 1.173e-011 3.556e-012 7.912e-013 3.297e-014 9.330e-015 0.000e+000 5.222e-005 4.793e-007 2.926e-014 8.364e-004 7.770e-005 5.780e-005 4.000e-008 3.362e-010 2.228e-007 1.037e-007 5.141e-008 1.389e-008 2.328e-009	5.574e-011 2.252e-011 8.569e-012 2.355e-014 8.689e-013 1.299e-017 2.662e-015 3.503e-007 3.214e-014 2.511e-004 8.533e-005 4.225e-005 4.239a-008 2.457e-010 5.917e-088 7.581e-088 3.757e-088 1.525e-089	-10.118 -10.511 -10.931 -11.449 -12.102 -13.482 -14.030 -44.396 -4.282 -6.319 -13.534 -3.078 -4.110 -4.238 -7.398 -9.473 -6.652 -6.984 -7.289 -7.857 -8.633	-10.254 -10.647 -11.067 -13.628 -12.061 -16.886 -14.575 -44.355 -44.355 -4.464 -6.456 -13.493 -3.600 -4.069 -4.374 -7.357 -9.610 -7.228 -7.120 -7.425 -7.817 -8.592
Percent error 	II Mass Total alkal Total Total Total Total Total Total Total Total Species H+ CH- H2O 0.0000+000 CH4 1.339e-001 CC2 CHC3- CAHC03+ MgHC03+ Fe_diHC03 CO3-2 Fe_diC03	mic strength f water (kg) inity (eq/kg) CO2 (mol/kg) CO2	- 0.39 - 0.39 - 0.000-0 - 1.000-0 - 2.967-0 - 2.967-0 - 2.507 - 2.500 - 2.300 - 2.500 - 2.300 - 2.500 - 2.300 - 2.500 - 2.300 - 2.300 - 2.300 - 2.500 - 2.300 - 2.500 - 2.300 - 2.500 - 2.500	01 00 02 11 14 +002 +001 Molality -5.322 -8.382 1.744 -141.384 -0.962 -1.690 -2.040 -4.238 -4.288 -5.068 -5.663 -6.127 -6.980	Log Activity -5.434 -8.569 -0.004 -141.344 -0.921 -1.842 -2.193 -4.374 -4.424 -4.968 -5.622 -6.737 -6.939	$\begin{array}{c} -0.136\\ -0.136\\ -0.136\\ -2.179\\ 0.041\\ -3.405\\ -0.545\\ H(0)\\ 0.041\\ K\\ -0.181\\ -0.136\\ 0.041\\ My\\ -0.523\\ 0.041\\ -0.136\\ 0.041\\ -0.136\\ 0.041\\ -0.136\\ -0.136\\ -0.136\\ -0.136\\ -0.136\\ -0.136\\ -0.136\\ -0.136\\ 0.041$	Fe_tri(12+ Fe_tri(12+ Fe_tri(304)2- Fe_tri2(0+)2+4 Fe_tri3(0+)4+5 Fe_triHSD4+2 0.000e+000 H2 5.270e-005 K+ KSO4- KCH 9.719e-004 Mg+20 Mg504 Mg504 Mg503 Mg603+ Mg703+ Mg70+	7.627e-011 3.081e-011 1.173e-011 3.556e-012 7.912e-013 3.297e-014 9.330e-015 0.000e+000 5.222e-005 4.793e-007 2.926e-014 8.364e-004 7.770e-005 5.780e-005 4.000e-008 3.362e-010 2.228e-007 1.037e-007 5.141e-008 1.389e-008 2.328e-009 7.845e-010	5.574e-011 2.252e-011 8.569e-012 2.355e-014 8.689e-013 1.299e-017 2.662e-015 3.502e-007 3.214e-010 2.511e-004 8.533e-005 4.225e-005 4.239a-008 2.457e-010 5.917e-008 7.581e-008 3.757e-008 1.525e-009 8.615e-010	-10.118 -10.511 -10.931 -11.449 -12.102 -13.482 -14.030 -44.396 -4.282 -6.319 -13.534 -3.078 -4.110 -4.238 -7.398 -9.473 -6.652 -6.984 -7.289 -7.857 -8.633 -9.105	-10.254 -10.647 -11.067 -13.628 -12.061 -16.886 -14.575 -44.355 -44.355 -4.464 -6.456 -13.493 -3.600 -4.069 -4.374 -7.357 -9.610 -7.228 -7.120 -7.425 -7.817 -8.592 -9.065
Percent error  Log Gemma -0.113 -0.187 0.000 C(-4) 0.041 -0.152 -0.152 -0.152 -0.136 0.041 0.052 0.055 0.055 0.055 0.055 0.055 0.055 0.055 0.055 0.055 0.055 0.055 0.057 0.055 0.055 0.041 0.041 0.041 0.041 0.041 0.055 0.055 0.055 0.055 0.055 0.055 0.041 0.041 0.041 0.041 0.041 0.041 0.055 0.055 0.055 0.055 0.041 0.041 0.041 0.041 0.041 0.041 0.055	II MESS Total alkali Total	mic strength f water (kg) inity (eq/kg) CO2 (mol/kg) CO2	- 0.39 - 0.39 - 0.000-0 - 1.000-0 - 2.967-0 - 2.967-0 - 2.507 - 2.508-0 - 0.00 - 2.508-0 - 0.00 - 47 - 0.00 - 0.00 - 47 - 0.00 - 0.00 - 47 - 0.00 - 0.	01 00 02 11 14 +002 +001 Molality -5.322 -8.382 1.744 -141.384 -0.962 -1.690 -2.040 -4.238 -4.288 -5.068 -5.663 -6.127 -6.980 -6.984	Log Activity -5.434 -8.569 -0.004 -141.344 -0.921 -1.842 -2.193 -4.374 -4.424 -4.968 -5.622 -6.737 -6.939 -7.120	$\begin{array}{c} -0.136\\ -0.136\\ -0.136\\ -2.179\\ 0.041\\ -3.405\\ -0.545\\ H(0)\\ 0.041\\ K\\ -0.181\\ -0.136\\ 0.041\\ My\\ -0.523\\ 0.041\\ -0.136\\ 0.041\\ -0.136\\ 0.041\\ -0.136\\ 0.041$	Fe_tri(12+ Fe_tri(12+ Fe_tri(304)2- Fe_tri2(0+)2+4 Fe_tri2(0+)2+4 Fe_tri3(0+)4+5 Fe_triHS04+2 0.000e+000 H2 5.270e-005 K+ KS04- KCH 9.719e-004 Mg+20 Mg504 Mg504 Mg504 Mg503 Mg603+ Mg504 Mg503 Mg603+ Mg703+	7.627e-011 3.081e-011 1.173e-011 3.556e-012 7.912e-013 3.297e-014 9.330e-015 0.000e+000 5.222e-005 4.793e-007 2.926e-014 8.364e-004 7.770e-005 5.780e-005 4.000e-008 3.362e-010 2.228e-007 1.037e-007 5.141e-008 1.389e-008 2.328e-009 7.845e-010 1.502e-010	5.574e-011 2.252e-011 8.569e-012 2.355e-014 8.689e-013 1.299e-017 2.662e-015 3.602e-015 3.503e-007 3.214e-014 2.511e-004 8.533e-005 4.225e-005 4.239a-008 2.457e-010 5.917e-088 7.581e-088 3.757e-088 1.525e-089 8.615e-010 1.098e-010	-10.118 -10.511 -10.931 -11.449 -12.102 -13.482 -14.030 -44.396 -4.282 -6.319 -13.534 -3.078 -4.110 -4.238 -7.398 -9.473 -6.652 -6.984 -7.289 -7.857 -8.633 -9.105 -9.823	-10.254 -10.647 -11.067 -13.628 -12.061 -16.886 -14.575 -44.355 -44.355 -4.464 -6.456 -13.493 -3.600 -4.069 -4.374 -7.357 -9.610 -7.228 -7.120 -7.425 -7.817 -8.592 -9.065 -9.959
Percent error  Log Gemma -0.113 -0.187 0.000 C(-4) 0.041 -0.152 -0.152 -0.152 -0.136 0.041	IIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIII	mic strength for water (kg) imity (eq/kg) CO2 (mol/kg) CO2 (mol/kg) CO	- 0.39 - 0.39 - 0.000+0 - 1.000+0 - 2.967-0 - 2.967-0 - 2.507-0 - 2.355-0 - 0.007-0 - 1.516-007 - 7.5816-008 - 4.393e-008	01 00 02 01 14 +002 +001 Molality -5.322 -8.382 1.744 -0.962 -1.690 -2.040 -4.238 -4.288 -5.068 -5.663 -6.127 -6.980 -6.964 -7.398	Log Activity -5.434 -8.569 -0.004 -141.344 -0.921 -1.842 -2.193 -4.374 -4.424 -4.968 -5.622 -6.737 -6.939 -7.120 -7.357	$\begin{array}{c} -0.136\\ -0.136\\ -0.136\\ -2.179\\ 0.041\\ -3.405\\ -0.545\\ H(0)\\ 0.041\\ K\\ -0.181\\ -0.136\\ 0.041\\ Mg\\ -0.523\\ 0.041\\ -0.136\\ 0.041\\ -0.136\\ 0.041\\ -0.136\\ Mn(2)\\ -0.576\\ -0.136\\ -0.136\\ 0.041\\ 0.041\\ 0.041\\ 0.041\\ -0.136\\ 0.041\\ 0.041\\ -0.136\\ 0.041\\ 0.041\\ -0.136\\ 0.041\\ 0.041\\ -0.136\\ 0.041\\ -0.136\\ 0.041\\ 0.041\\ -0.136\\ 0.041\\ 0.041\\ -0.136\\ -0.041\\ -0.041\\ -0.041\\ -0.041\\ -0.041\\ -0.040\\ -0.$	Fe_tri(12+ Fe_tri(12+ Fe_tri(304)2- Fe_tri2(0+)2+4 Fe_tri3(0+)4+5 Fe_triHS04+2 0.0000+000 H2 5.2700=005 K+ KS04- KCH 9.7190=004 Mg+2 Mg504 Mg504 Mg503 Mg604+ 3.951e=007 Mx+2 Mg504 Mg603+ Mg603 Mg604+ 3.951e=007 Mx+2 Mx+03+ MxCl+ Mx504 MxCl2 Mx603 MxCl3- Mx604+ Mx603 Mx613- Mx604+ Mx604 Mx603 Mx613- Mx604 Mx764	7.627e-011 3.081e-011 1.173e-011 3.556e-012 7.912e-013 3.297e-014 9.330e-015 0.000e+000 5.222e-005 4.793e-007 2.926e-014 8.364e-004 7.770e-005 5.780e-005 4.000e-008 3.362e-010 2.228e-007 1.037e-007 5.141e-008 1.389e-008 2.328e-009 7.845e-010 1.502e-010 5.607e-013	5.574e-011 2.252e-011 8.569e-012 2.355e-014 8.689e-013 1.299e-017 2.662e-015 3.503e-007 3.214e-014 2.511e-004 8.533e-005 4.225e-005 4.253e-007 5.917e-008 7.581e-008 3.757e-008 1.525e-008 8.615e-010 1.098e-010	-10.118 -10.511 -10.931 -11.449 -12.102 -13.482 -14.030 -44.396 -4.282 -6.319 -13.534 -3.078 -4.110 -4.238 -7.398 -9.473 -6.652 -6.984 -7.289 -7.857 -8.633 -9.105 -9.823 -12.251	-10.254 -10.647 -11.067 -13.628 -12.061 -16.886 -14.575 -44.355 -44.355 -44.355 -4.464 -6.456 -13.493 -3.600 -4.069 -4.374 -7.357 -9.610 -7.228 -7.120 -7.228 -7.120 -7.425 -7.817 -8.592 -9.065 -9.959 -12.387
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Percent error Log Gamma -0.113 -0.187 0.000 C(-4) 0.041 -0.152 -0.152 -0.152 -0.136 0.041 0.041 -0.610 0.041 -0.136 0.041 -0.136	I I I I I I I I I I I I I I I I I I I	mic strength for water (kg) inity (eq/kg) CO2 (mol/kg) CO2 (mol/kg) CO	- 0.39 - 0.39 - 0.000 - 1.0000-0 - 2.967-0 - 2.967-0 - 2.507-0 - 2.507-0 - 2.500 - 2.3050 - 0.000 -	01 00 02 01 14 +002 +001 Molality -5.322 -8.382 1.744 -0.962 -1.690 -2.040 -4.238 -4.288 -5.068 -5.663 -6.127 -6.980 -6.984 -7.398 -8.861 -9.105	Log Activity -5.434 -8.569 -0.004 -141.344 -0.921 -1.842 -2.193 -4.374 -4.424 -4.968 -5.622 -6.737 -6.939 -7.120 -7.357 -8.997 -9.065	-0.136 -0.136 -2.179 0.041 -3.405 -0.545 H(0) 0.041 K -0.181 -0.136 0.041 Mg -0.523 0.041 -0.136 0.041 -0.136 Mn(2) -0.576 -0.136 -0.136 0.041 0.041 0.041 -0.136 -0.136 Mn(3) -0.136	Fe_tri(12+ Fe_tri(12+ Fe_tri(304)2- Fe_tri2(0+)2+4 Fe_tri3(0+)4+5 Fe_triHS04+2 0.0000+000 H2 5.2700=005 K+ KS04- KCH 9.7190=004 Mg+2 Mg504 Mg	7.627e-011 3.081e-011 1.173e-011 3.556e-012 7.912e-013 3.297e-014 9.330e-015 0.000e+000 5.222e-005 4.793e-007 2.926e-014 8.364e-004 7.770e-005 5.780e-005 4.000e-008 3.362e-010 2.228e-007 1.037e-007 5.141e-008 1.389e-008 2.328e-009 7.845e-010 1.502e-010 5.607e-013 4.528e-017	5.574e-011 2.252e-011 8.569e-012 2.355e-014 8.689e-013 1.299e-017 2.662e-015 3.503e-007 3.214e-014 2.511e-004 8.533e-007 4.225e-005 4.393e-008 2.457e-010 5.917e-008 7.581e-008 3.757e-008 1.557e-009 8.615e-010 1.098e-013 2.693e-018	-10.118 -10.511 -10.931 -11.449 -12.102 -13.482 -14.030 -44.396 -4.282 -6.319 -13.534 -3.078 -4.110 -4.238 -7.398 -9.473 -6.652 -6.984 -7.289 -7.857 -8.633 -9.105 -9.823 -12.251 -16.344	-10.254 -10.647 -11.067 -13.628 -12.061 -16.886 -14.575 -44.355 -44.355 -4.464 -6.456 -13.493 -3.600 -4.069 -4.374 -7.357 -9.610 -7.228 -7.120 -7.228 -7.120 -7.425 -7.817 -8.592 -9.065 -9.959 -12.387 -17.570
Percent error Log Gamma -0.113 -0.187 0.000 C(-4) 0.041 -0.152 -0.152 -0.152 -0.136 0.041 0.041 -0.610 0.041 -0.136 0.041 -0.136 0.041 -0.136 0.041 -0.136 0.041	I I I I I I I I I I I I I I I I I I I	mic strength for water (kg) inity (eq/kg) CO2 (mol/kg) CO2 (mol/kg) CO	- 0.39 - 0.39 - 0.000 - 1.0000-0 - 2.967-0 - 2.967-0 - 2.507-0 - 2.507 - 2.508-0 - 0.00 - 47 - Activity 3.678e-006 2.698e-009 9.911e-001 0.000e+000 1.200e-001 1.438e-002 6.417e-003 4.256-005 1.077e-005 2.385e-006 1.833e-007 1.518-007 1.518-007 8.615e-010	01 00 02 01 14 +002 +001 Molality -5.322 -8.382 1.744 -0.962 -1.690 -2.040 -4.238 -4.288 -5.068 -5.663 -6.127 -6.980 -6.984 -7.398 -8.861 -9.105	Log Activity -5.434 -8.569 -0.004 -141.344 -0.921 -1.842 -2.193 -4.374 -4.424 -4.968 -5.622 -6.737 -6.939 -7.120 -7.357 -8.997 -9.065	-0.136 -0.136 -2.179 0.041 -3.405 -0.545 H(0) 0.041 K -0.181 -0.136 0.041 Mg -0.523 0.041 -0.136 0.041 -0.136 Mn(2) -0.576 -0.136 -0.136 0.041 0.041 0.041 0.041 0.041 -0.136 Mn(3) -1.226 Na	Fe_tri(12+ Fe_tri(12+ Fe_tri(304)2- Fe_tri2(0+)2+4 Fe_tri3(0+)4+5 Fe_triHS04+2 0.0000+000 H2 5.2700=005 K+ KS04- KCH 9.7190=004 Mg+2 Mg504 Mg504 Mg504 Mg503 MgCH+ 3.9510=007 Mx+2 Mx504 MxCl MxCl MxCl MxCl 4.5280=017 Mx+3 4.1830=004 Nat	7.627e-011 3.081e-011 1.173e-011 3.556e-012 7.912e-013 3.297e-014 9.330e-015 0.000e+000 5.222e-005 4.793e-007 2.926e-014 8.364e-004 7.770e-005 5.780e-005 4.000e-008 3.362e-010 2.228e-007 1.037e-007 5.141e-008 1.389e-008 2.328e-009 7.845e-010 1.502e-010 5.607e-013 4.528e-017 4.132e-004	5.574e-011 2.252e-011 8.569e-012 2.355e-014 8.689e-013 1.299e-017 2.662e-015 3.503e-007 3.214e-014 2.511e-004 8.533e-005 4.225e-005 4.393e-008 2.457e-010 5.917e-008 7.571e-008 3.757e-008 8.615e-010 1.098e-013 2.693e-018 2.250e-004	-10.118 -10.511 -10.931 -11.449 -12.102 -13.482 -14.030 -44.396 -4.282 -6.319 -13.534 -3.078 -4.110 -4.238 -7.398 -9.473 -6.652 -6.984 -7.289 -7.857 -8.633 -9.105 -9.823 -12.251 -16.344 -3.384	-10.254 -10.647 -11.067 -13.628 -12.061 -16.886 -14.575 -44.355 -44.355 -4.464 -6.456 -13.493 -3.600 -4.069 -4.374 -7.357 -9.610 -7.228 -7.120 -7.228 -7.120 -7.425 -7.817 -8.592 -9.065 -9.959 -12.387 -17.570 -3.530
Percent error Log Gamma -0.113 -0.187 0.000 C(-4) 0.041 -0.152 -0.152 -0.136 0.041 0.041 -0.610 0.041 -0.610 0.041 -0.136 0.058 -0.5588 -0.558	I I I I I I I I I I I I I I I I I I I	mic strength five terrength (e) water (kg) (m1/kg) (c2 (m1/kg) (c2 (m1/kg)) (c2 (m2/kg) (c2 (m2/kg)) (c2 (	- 0.39 - 0.39 - 0.000 - 1.0000-0 - 2.967-0 - 2.967-0 - 2.507-0 - 2.507-0 - 2.508-0 - 0.00 - 47 - Activity 3.678e-006 2.698e-009 9.911e-001 0.000e+000 1.200e-001 1.438e-002 6.417e-003 4.275e-005 1.077e-005 2.385e-006 1.833e-007 1.518-007 1.518-007 3.4398e-002 3.498e-002	01 00 02 11 14 +002 +001 Molality -5.322 -8.382 1.744 -0.962 -1.690 -2.040 -4.238 -4.288 -5.068 -5.663 -6.127 -6.980 -6.984 -7.398 -8.861 -9.105 -9.105 -0.889	Log Activity -5.434 -8.569 -0.004 -141.344 -0.921 -1.842 -2.193 -4.374 -4.424 -4.968 -5.622 -6.737 -6.939 -7.120 -7.357 -8.997 -9.065 -1.456	$\begin{array}{c} -0.136\\ -0.136\\ -2.179\\ 0.041\\ -3.405\\ -0.545\\ H(0)\\ 0.041\\ K\\ -0.181\\ -0.136\\ 0.041\\ Mg\\ -0.523\\ 0.041\\ -0.136\\ 0.041\\ -0.136\\ 0.041\\ -0.136\\ 0.041\\ -0.136\\ -0.136\\ -0.136\\ -0.136\\ 0.041\\ 0.041\\ 0.041\\ 0.041\\ -0.136\\ Mn(3)\\ -1.226\\ Na\\ \end{array}$	Fe_tri(12+ Fe_tri(12+ Fe_tri(304)2- Fe_tri2(0+)2+4 Fe_tri3(0+)4+5 Fe_triHS04+2 0.0000+000 H2 5.2700-005 K+ KS04- KCH 9.7190-004 Mg+2 Mg504	7.627e-011 3.081e-011 1.173e-011 3.556e-012 7.912e-013 3.297e-014 9.330e-015 0.000e+000 5.222e-005 4.793e-007 2.926e-014 8.364e-004 7.770e-005 5.780e-005 4.000e-008 3.362e-010 2.228e-007 1.037e-007 5.141e-008 1.389e-008 2.328e-009 7.845e-010 1.502e-010 5.607e-013 4.528e-017 4.132e-004 2.933e-005	5.574e-011 2.252e-011 8.569e-012 2.355e-014 8.689e-013 1.299e-017 2.662e-015 3.503e-007 3.214e-014 2.511e-004 8.533e-005 4.225e-005 4.257e-000 5.917e-008 7.57e-008 3.757e-008 1.557e-009 8.615e-010 1.098e-013 2.693e-018 2.950e-004 2.142e-005	-10.118 -10.511 -10.931 -11.449 -12.102 -13.482 -14.030 -44.396 -4.282 -6.319 -13.534 -3.078 -4.110 -4.238 -7.398 -9.473 -6.652 -6.984 -7.289 -7.857 -8.633 -9.105 -9.823 -12.251 -16.344 -3.384 -5.533	-10.254 -10.647 -11.067 -13.628 -12.061 -16.886 -14.575 -44.355 -44.355 -4.464 -6.456 -13.493 -3.600 -4.069 -4.374 -7.357 -9.610 -7.228 -7.120 -7.425 -7.817 -8.592 -9.065 -9.959 -12.387 -17.570 -3.530 -5.669

0.041	NaHCO3	2.172e-006	2.385e-006	-5.663	-5.622
-0.136	NaCO3-	1.378e-009	1.007e-009	-8.861	-8.997
0.041	NaCH	4.783e-013	5.253e-013	-12.320	-12.280
O(0)	3.828e-004 02	1.914e-004	2.102e-004	-3.718	-3.677
0.041 S(-2)	0.000e+000	0.000-000	0.000-000	127 062	127 001
0.041	HZ5	0.000e+000	0.000e+000	130 2/1	130 /20
-0.187	e 2	0.000+000	0.000-000	146 277	1/6 012
-0.635	E di (HS) 2	0.000e+000	0.000=+000	_274 530	_274_489
0.041	Fe di (HS)3-	0.000e+000	0.000e+000	-411.744	-411.880
-0.136 S(6)	1.579e-002				
0.041	Ca904	9.212e-003	1.012e-002	-2.036	-1.995
-0.651	904-2	6.490e-003	1.449e-003	-2.188	-2.839
0.041	MgSO4	7.770e-005	8.533e-005	-4.110	-4.069
0.041	Fe_di.904	6.143e-006	6.746e-006	-5.212	-5.171
-0.136	NaSO4-	2.933e-006	2.143e-006	-5.533	-5.669
-0.136	H904-	7.092e-007	5.183e-00/	-6.149	-6.285
-0.136	K904-	4.793e-007	3.503e-007	-6.319	-6.456
-0.136	CaHSO4+	2.983e-007	2.180e-007	-6.525	-6.662
0.041	MnS04	1.389e-008	1.525e-008	-7.857	-7.817
-0.136	Fe_triso4+	3.6986-010	2.702e-010	-9.432	-9.568
-0.136	Fe_CIHSU4+	2.232e-010	1.6310-010	-9.651	-9.788
-0.136	Fe_tr1 (504) 2-	1.1/3e-011	8.569e-012	-10.931	-11.06/
-0.545	Fe_tr1H904+2	9.330e-015	2.662e-015	-14.030	-14.5/5
		-Saturation i	ndiæs		
		or 1 -			
	Mase		AP 100 KT	0-001	
	Aragonite Calcite Calcite CC2(g) Dolomite Gypsun H2(g) H20(g) H20(g) H20(g) Haismernite Marganite C2(g) Pyrochroite Pyrolosite Rindochrosite Sulfar	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	CaCO3 CACO3 CH4 CC2 CaMg(CO3)2 CaSO4:2H2O H2O H2O H2O H2O M3O4 MnOCH O2 Mn(CH)2 MnO2 S	
Reaction ster	3	101.00 90.	12 4.00	5	
Using solutio Using pure pl Using kinetic	n 1. nase assemblage 1 ns 1. K	inetics defin	ed in simula	ation 2.	
Kinetics 1.	Kinetics define	d in simulati	an 2.		
	Time step: 3100	seconds (In	cremented t	ime: 3600 s	econds)
Coofficient	Rate name	Delta Moles	Total Moles	Reactant	
werndalt	Fe di ax	-2.162e-005	1.000e+000	Fe di	
-1		2.1020 000		Fe tri	
1					
		Phase asser	blage		
				Moles in as	semblage
Delta	Phase	SI log I	AP log KT	Initial	Final
E 40E- 00C	02 (g)	-0.79 -3.	68 -2.89	1.000e+001	1.000e+001-
5.405e-006		Solution com	ogition		
	Elements	Molality	Moles		
	C Ca	1.389e-001 1.476e-001	1.389e-001 1.476e-001		
	Cl Fe_di	2.367e-001 1.356e-004	2.367e-001 1.356e-004		
	Fe_tri K	2.542e-005 5.270e-005	2.542e-005 5.270e-005		
	Mg Min	9.719e-004 3.951e-007	9.719e-004 3.951e-007		
	Na S	4.183e-004 1.579e-002	4.183e-004 1.579e-002		
	I	escription of	solution		

		pH pe	= 5.434 = 15.169	Charge Adjust	e balance ed to redox
equilibrium	Activ	ity of water	= 0.991		
	Ion Mass o	nic strength E water (kg)	= 4.068e-0 = 1.000e+0	001 000	
	Total alkalin Total (	nity (eg/kg) 302 (mol/kg)	= 2.970e-0 = 1.389e-0	)02 )01	
	Tenperal Electrical I	ture (deg C) balance (eg)	= 25.000 = 2.519e-0	)14	
Percent erro	or, 100*(Cat- An	Iterations	= 0.00 = 44 = 1.110421c		
		Total 0	= 5.587724	+002	
	D	istribution c	f species		
				Log	Log
Log	Species	Molality	Activity	Molality	Activity
Ganma					
-0.113	H+	4.7/0e-006	3.681e-006	-5.321	-5.434
-0.187	UH- 170	4.151e-009	2.6968-009	-8.382	-8.569
0.000	0.000-+000	3.3316+001	9.9118-001	1.744	-0.004
0.041	CH4	0.000e+000	0.000e+000	-141.384	-141.344
C(4)	1.389e-001 CO2	1.093e-001	1.200e-001	-0.962	-0.921
0.041	H003-	2.041e-002	1.437e-002	-1.690	-1.843
-0.152	CaHCO3+	9.111e-003	6.414e-003	-2.040	-2.193
-0.152	MgHCO3+	5.778e-005	4.223e-005	-4.238	-4.374
-0.136	Fe_diH003+	4.440e-005	3.245e-005	-4.353	-4.489
-0.136	CaCO3	9.798e-006	1.076e-005	-5.009	-4.968
0.041	NaHCO3	2.171e-006	2.384e-006	-5.663	-5.623
-0.610	003-2	7.456e-007	1.831e-007	-6.128	-6.737
-0.136	MnHCO3+	1.037e-007	7.579e-008	-6.984	-7.120
0.041	Fe_diCO3	9.031e-008	9.917e-008	-7.044	-7.004
0.041	MgCO3	3.995e-008	4.388e-008	-7.398	-7.358
-0.136	NaCO3-	1.376e-009	1.006e-009	-8.861	-8.997
0.041	MinCO3	7.837e-010	8.606e-010	-9.106	-9.065
Ca	1.476e-001 Ca+2	1.293e-001	3.498e-002	-0.889	-1.456
-0.568	CaSO4	9.213e-003	1.012e-002	-2.036	-1.995
_0 152	CaHCO3+	9.111e-003	6.414e-003	-2.040	-2.193
0.041	CaCO3	9.798e-006	1.076e-005	-5.009	-4.968
-0.136	CaHSO4+	2.985e-007	2.182e-007	-6.525	-6.661
-0.136	CaOH+	2.139e-009	1.563e-009	-8.670	-8.806
Cl	2.367e-001 Cl-	2.367e-001	1.559e-001	-0.626	-0.807
-0.181	Fe_diCl+	6.648e-006	4.859e-006	-5.177	-5.313
-0.136	MnCl+	5.142e-008	3.758e-008	-7.289	-7.425
-0.136	MnCl2	2.329e-009	2.557e-009	-8.633	-8.592
_0.545	Fe_triCl+2	1.879e-009	5.362e-010	-8.726	-9.271
-0.136	Fe_triCl2+	5.109e-010	3.733e-010	-9.292	-9.428
-0.136	MnCl3-	1.502e-010	1.098e-010	-9.823	-9.959
0.041	Fe_triCl3	5.300e-012	5.820e-012	-11.276	-11.235
Fe_di	1.356e-004 Fe_di+2	7.915e-005	2.258e-005	-4.102	-4.646
-0.545	Fe_diH003+	4.440e-005	3.245e-005	-4.353	-4.489
-0.136	Fe_diCl+	6.648e-006	4.859e-006	-5.177	-5.313
-0.136	Fe_di304	5.300e-006	5.820e-006	-5.276	-5.235
0.041	Fe_diCO3	9.031e-008	9.917e-008	-7.044	-7.004
-0.136	Fe_diOH+	2.631e-009	1.923e-009	-8.580	-8.716
-0.136	Fe_diH904+	1.927e-010	1.408e-010	-9.715	-9.851
0.041	Fe_di(HS)2	0.000e+000	0.000e+000	-274.593	-274.553
-0.136	Fe_di (HS) 3-	0.000e+000	0.000e+000	-411.808	-411.944
Fe_tri	2.542e-005 Fe_tri(OH)2+	2.416e-005	1.766e-005	-4.617	-4.753
-0.136	Fe_triOH+2	6.941e-007	1.980e-007	-6.159	-6.703
-0.545	Fe_tri(OH)3	5.577e-007	6.125e-007	-6.254	-6.213
_0 136	Fe_triSO4+	2.477e-009	1.810e-009	-8.606	-8.742
-1.226	Fe_tri+3	1.915e-009	1.139e-010	-8.718	-9.944

I

	Anhydrite Aragonite Calcite CH4(g)	0.07 -4. 0.14 -8. 0.29 -8. -138.48 -141.	29 -4.36 19 -8.34 19 -8.48 34 -2.86	Ca904 Ca003 Ca003 CH4	
	Phase	SI log I	AP log KT		
	79		1		
		-Saturation i	ndices		
-0.545	Fe_triH904+2	6.254e-014	1.784e-014	-13.204	-13.749
-0.136	Fe_tri(SO4)2-	7.854e-011	5.740e-011	-10.105	-10.241
-0.136	Fe_diH904+	1.927e-010	1.408e-010	-9.715	-9.851
-0.136	Fe_tri904+	2.477e-009	1.810e-009	-8.606	-8.742
0.041	MnSO4	1.389e-008	1.525e-008	-7.857	-7.817
-0.136	CaHSO4+	2.985e-007	2.182e-007	-6.525	-6.661
-0.136	K904-	4.793e-007	3.503e-007	-6.319	-6.456
-0.136	H904-	7.097e-007	5.187e-007	-6.149	-6.285
-0.136	NaSO4-	2.933e-006	2.143e-006	-5.533	-5.669
0.041	Fe_diSO4	5.300e-006	5.820e-006	-5.276	-5.235
0.041	Mg904	7.770e-005	8.533e-005	-4.110	-4.069
-0.651	SO4-2	6.490e-003	1.449e-003	-2.188	-2.839
0.041	Ca904	9.213e-003	1.012e-002	-2.036	-1.995
-0.136 5(6)	ге <u>с</u> ц (н5) <i>3</i> - 1.579е-002	v.uue+uuu	v.uue+uuu	-411.808	-411.944
0.041	re_ou(H5)2	0.000-000	0.000~000	_2/4.593	-2/4.553
-0.635	u-2	0.000-000	0.000~:000	274 502	-140.912
-0.187	s_2		0.000=+000	-1/6 241	-1/6 017
0.041	HS_		0.000~+000	-130 2/1	-139 //20
0.041 S(-2)	 0.000e+000	0.000-:000	0.000~000	_127 0.01	_127_001
0.041 D(0)	3.828e-004	1 914-004	2 102-004	-3 718	-3 677
-0.136	NaOH	4.780e-013	5.249e-013	-12.321	-12.280
0.041	NaCO3-	1.376e-009	1.006e-009	-8.861	-8.997
-0.136	NaHCO3	2.171e-006	2.384e-006	-5.663	-5.623
-0.146	NaSO4-	2.933e-006	2.143e-006	-5.533	-5.669
-1.220 Na	4.183e-004 Na+	4.132e-004	2.950e-004	-3.384	-3.530
Mn(3)	4.532e-017 Mn+3	4.532e-017	2.696e-018	-16.344	-17.569
-0.136	MnCH+	5.604e-013	4.096e-013	-12.251	-12.388
-0.136	MnCl3-	1.502e-010	1.098e-010	-9.823	-9.959
0.041	MnCO3	7.837e-010	8.606e-010	-9.106	-9.065
0.041	MnCl2	2.329e-009	2.557e-009	-8.633	-8.592
0.041	MnSO4	1.389e-008	1.525e-008	-7.857	-7.817
-0.136	MnCl+	5.142e-008	3.758e-008	-7.289	-7.425
-0.136	MnHCO3+	1.037e-007	7.579e-008	-6.984	-7.120
-0.576	3.951e-00/ Mn+2	2.228e-007	5.917e-008	-6.652	-7.228
-0.136	MgCH+	3.359e-010	2.455e-010	-9.474	-9.610
0.041	MgCO3	3.995e-008	4.388e-008	-7.398	-7.358
-0.136	MgHCO3+	5.778e-005	4.223e-005	-4.238	-4.374
0.041	Mg904	7.770e-005	8.533e-005	-4.110	-4.069
Mg -0.523	9.719e-004 Mg+2	8.364e-004	2.511e-004	-3.078	-3.600
0.041	KOH	2.924e-014	3.211e-014	-13.534	-13.493
-0.136	K904-	4.793e-007	3.503e-007	-6.319	-6.456
-0.181	5.270€-005 K+	5.222e-005	3.440e-005	-4.282	-4.464
0.041	H2	0.000e+000	0.000e+000	-44.396	-44.355
-0.545 H(0)	Fe_tr1H904+2	6.254e-014	1.784e-014	-13.204	-13.749
0.041	Fe_triCL3	5.300e-012	5.820e-012	-11.2/6	-11.235
-3.405	Fe_tri3(OH)4+5	9.880e-012	3.893e-015	-11.005	-14.410
-0.136	Fe_tri (904)2-	7.854e-011	5.740e-011	-10.105	-10.241
-2.179	Fe_tri2(OH)2+4	1.593e-010	1.055e-012	-9.798	-11.977
-0.136	Fe_tri (OH) 4-	2.058e-010	1.504e-010	-9.687	-9.823
-0.136	Fe_triCl2+	5.109e-010	3.733e-010	-9.292	-9.428
-0.545	Fe_triCi+2	1.8/9e-009	5.362e-010	-8.726	-9.2/1

Reaction ste	CC2(g) Dolamite Opesum H2(g) H2S(g) H2S(g) Halite Hausmanite C2(g) Pyrodraoite Pyrodraoite Rhododraoite Sulfur p 4.	$\begin{array}{ccccccc} 0.55 & -0.\\ -1.44 & -18.\\ 0.28 & -4.\\ -41.21 & -44.\\ -1.51 & -0.\\ -136.92 & -137.\\ -5.92 & -4.\\ -8.92 & 52.\\ -1.10 & 24.\\ -0.79 & -2.\\ -1.10 & 24.\\ -0.79 & -3.\\ -1157 & 3.\\ -1.57 & 3.\\ -1.64 & -4.\\ -2.84 & -13.\\ -101.60 & -96.\\ \end{array}$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	CC2 CaMg(CC3)2 CaSO4:2H2C H2 H2O H2S NaC1 Mn3O4 Mn3O4 Mn3O4 Mn3O4 Mn(CH)2 Mn(CH)2 Mn02 S	
Using soluti Using pure p Using kineti	on 1. hase assemblage 1 cs 1. K	l. inetics defin	ed in simula	tion 2.	
Kinetics 1.	Kinetics define	d in simulati	an 2.		
	Time step: 1080	0 seconds (I	incremented t	ime: 14400	seconds)
Coefficient	Rate name	Delta Moles	Total Moles	Reactant	
-1	Fe_di_ax	-5.450e-005	9.999e-001	Fe_di	
1				Fe_tri	
			blage		
		111450 (4560)	Linge		
Delta	Phase	SI log I	M AP log KT	bles in as Initial	semblage Final
1.363e-005	O2 (g)	-0.79 -3.	68 -2.89 1	.000e+001	1.000e+001-
		-Solution comp	osition		
	Elements	Molality	Moles		
	C Ca	1.389e-001 1.476e-001	1.389e-001 1.476e-001		
	Cl Fe_di	2.367e-001 8.109e-005	2.36/e-001 8.109e-005		
	Fe <u>t</u> ri K	7.991e-005 5.270e-005	7.991e-005 5.270e-005		
	Mg Mn	9.719e-004 3.951e-007	9.719e-004 3.951e-007		
	Na S	4.183e-004 1.579e-002	4.183e-004 1.579e-002		
	I	Description of	solution		
			5 422	đ	
		pH pe	= 5.433 = 15.169	Charge Adjust	e balance ed to redox
equilibrium	Activ	pH pe rity of water	= 5.433 = 15.169 = 0.991	Charge Adjust	e balance ed to redox
equilibrium	Activ Ic Mass c	pH pe nicy of water nic strength of water (kg)	= 5.433 = 15.169 = 0.991 = 4.067e-0 = 1.000e+0	Charge Adjust 001	e balance red to redox
equilibrium	Activ Io Mass c Total alkali Total	pH pe nicy of water nic strength f water (kg) nity (eg/kg) CO2 (mol/kg)	= 5.433 = 15.169 = 0.991 = 4.067e-0 = 1.000e+0 = 2.975e-0 = 1.389e-0	Charge Adjust 001 000 002 001	e balance ad to radax
equilibrium	Activ Ins Total alkali Total Tempera Electrical	pH pe nic strength of water (kg) nity (eg/kg) (CO2 (mol/kg) turre (deg C) balance (eg)	= 5.433 = 15.169 = 0.991 = 4.067e-C = 1.000e+C = 2.975e-C = 1.389e-C = 25.000 = 2.542e-C	Charge Adjust 001 002 001 114	e balance ed to redox
equilibrium Percent erro	Activ Ic Mass G Total alkali Total Temper Electrical or, 100* (Cat-]An	pH pe vity of water nic strength inty (eg/kg) CO2 (mol/kg) iture (deg C) balance (eg) )/(Cat+[An]) Iterations	= 5.433 = 15.169 = 0.991 = 4.067e-0 = 1.000e+0 = 2.975e-0 = 25.000 = 2.542e-0 = 0.00 = 34	Charge Adjust 001 002 001 114	e balance ed to redox
equilibrium Percent enro	Activ Ic Mass C Total alkali Total Tempera Electrical or, 100* (Cat-]An	pH pe nicy of water mic strength of water (kg) mity (cg/kg) c02 (mol/kg) thre (deg C) balance (cg) (C2 (mol/kg) threations Total H Total O	= 5.433 = 15.169 = 0.991 = 4.067e-C = 1.000e+C = 2.975e-C = 1.389e-C = 2.5.000 = 2.522e-C = 0.00 = 34 = 1.110421c = 5.5877266	Charge Adjust 001 000 002 001 114 \$+002 \$+001	e balance ed to redox
equilibrium Percent erro	Activ IR Mess c Total alkali Total Tempera Electrical or, 100* (Cat- An	pH pe nity of water nic strength of water (kg) nity (cg/kg) (C2 (ml/kg) three (cg) )/(Cat+ 2n]) Iterations Total 0 Distribution of	= 5.433 = 15.169 = 0.991 = 4.067e-C = 1.000erC = 2.975e-C = 25.000 = 2.542e-C = 0.00 = 34 = 1.110421e = 5.587726e	Charge Adjust 001 002 001 114 e+002 e+001	e balance ed to redox
equilibrium Percent enro	Activ Is Total alkali Total Tempera Electrical cr, 100* (Cat- An  -	pH pe nic strength of water (kg) 002 (mol/kg) 202 (mol/kg	= 5.433 = 15.169 = 0.991 = 4.067e-C = 1.000e+C = 2.575e-C = 0.00 = 2.542e-C = 0.00 = 34 = 1.110421e = 5.587726e	Charge Adjust 001 002 001 114 ++002 ++001	e balance ed to redox
equilibrium Percent erro  Log	Activ Is Total alkali Total Impera Electrical or, 100* (Cat- Aa	pH pe nic strength of water (kg) nity (cg/kg) CD2 (mol/kg) Dalance (cg) )/(Cat+[An]) Iterations Total H Total O Distribution c	= 5.433 = 15.169 = 0.991 = 4.067e-C = 1.000e+C = 2.975e-C = 25.000 = 2.542e-C = 0.00 = 34 = 1.110421e = 5.587726e	Charge Adjust 001 002 001 114 ++002 ++001 Log	e balance ed to redox I.og
equilibrium Percent erro  Log Gamma	Activ Is Mass of Total alkali Tempera Electrical cr, 100* (Cat- An  or, 100* (Cat- An	pH pe nic strength f water (kg) of (kg) (C2 (kg)	= 5.433 = 15.169 = 0.991 = 4.067e-0 = 1.000e0 = 2.975e-0 = 2.502e-0 = 0.00 = 34 = 1.110421e = 5.587726e ff species	Charge Adjust 001 002 001 010 114 ++002 ++001 Log Molality	e balance ad to radox I.og Activity
equilibrium Percent erro  Log Gamma -0.113	Activ Is Total alkali Total Total Tempera Electrical or, 100*(Cat- An  or, 100*(Cat- In  Species	pH pe vity of water mic strength of water (kg) CO2 (mol/kg) CO2 (mol/kg) Dialance (eq) Jolance (eq) Jolance (eq) Jolant H Total 0 Distribution of Molality 4.778e-006	= 5.433 = 15.169 = 0.991 = 4.067e-C = 1.000e4C = 2.975e-C = 2.975e-C = 25.000 = 34 = 1.110421e = 5.587726 of species	Charge Adjust 001 002 001 114 ++002 ++001 Log Molality -5.321	Log Activity -5.433
equilibrium Percent erro Log Gama -0.113 -0.187	Activ Is Total alkali Total Total Tempera Electrical or, 100*(Cat- An  or, 100*(Cat- An  Pactics Heter Species	pH pe rity of water mic strength of water (kg) (02 (mol/kg) (02 (mol/kg) balance (eq) )/(Cat+kal) Iterations Total H Total 0 Distribution of Molality 4.778e-006 4.143e-009	= 5.433 = 15.169 = 0.991 = 4.067e-C = 1.000e-C = 2.975e-C = 2.975e-C = 2.500 = 2.500 = 34 = 1.110421e = 5.587726 of species	Charge Adjust 001 002 001 114 ++002 ++001 Log Molality -5.321 -8.383	Log Activity -5.433 -8.570
equilibrium Percent erro Log Gamma -0.113 -0.187 0.000	Activ Is Total alkali Total alkali Total Tempera Electrical or, 100*(Cat- An  or, 100*(Cat- An  Papecies H+ CH- H2O	pH pe nity of water mic strength of water (kg) 022 (mol/kg) 022 (mol/kg) balance (eq) )/(Cat+An]) Iterations Total 0 Distribution of Molality 4.778e-006 4.143e-009 5.551e+001	= 5.433 = 15.169 = 0.991 = 4.067e-C = 1.000e-C = 1.389e-C = 2.975e-C = 2.502 = 0.00 = 34 = 1.110421e = 5.587726e of species Activity 3.687e-006 2.691e-009 9.911e-001	Charge Adjust 001 002 001 114 ++002 ++001 Molality -5.321 -8.383 1.744	Log Activity -5.433 -8.570 -0.004
equilibrium Percent erro  Log Gama -0.113 -0.187 0.000 C(-4) 0.001	Activ Ir Mass of Total alkali Total	pH pe rity of water mic strength fwater (kg) mity (eg/kg) 022 (mol./kg) three (cdg (C) fralarce (eg) //Cat+[An]) Iterations Total H Total O Oistribution of Molality 4.778e-006 4.143e-009 5.551e+001 0.000e+000	= 5.433 = 15.169 = 0.991 = 4.067e-C = 1.008-C = 2.975e-C = 1.383e-C = 2.502e-C = 0.00 = 34 = 1.110421e = 5.587726e of species Activity 3.687e-006 2.691e-009 9.911e-001	Charge Adjust 000 002 001 114 +002 +001 Log Molality -5.321 -8.383 1.744	E balance ed to redox Iog Activity -5.433 -8.570 -0.004 -141.343
equilibrium Percent erro 	Activ Is Mass of Total alkali Total	pH pe rity of water mic strength fwater (kg) mity (eg/kg) 022 (mol./kg) thure (deg C) palaroe (eg) //Cat+[An]) Iterations Total H Total O Distribution of Molality 4.778e-006 4.143e-009 5.551e+001 0.000e+000 1.093e-001	= 5.433 = 15.169 = 0.991 = 4.067e-C = 2.975e-C = 2.975e-C = 2.502e-C = 0.00 = 34 = 1.110421e = 5.587726e f species Activity 3.687e-006 2.691e-009 9.911e-001	Charge Adjust 001 002 001 114 +002 +001 Log Molality -5.321 -8.383 1.744 -141.384 -0.961	E balance ed to redox Iog Activity -5.433 -8.570 -0.004 -141.343 -0.921
equilibrium Percent error  Log Gamma -0.113 -0.187 0.000 C(-4) 0.001 C(4) 0.041	Activ Is Mass of Total alkali Total	pH pe rity of water mic strength fwater (kg) mity (eg/kg) 002 (mol/kg) three (eg C) relarce (eg C) rotal H Total 0 Distribution of Molality 4.778e-006 4.143e-009 5.551e+001 0.000e+000 1.093e-001 2.039e-002	= 5.433 = 15.169 = 0.991 = 4.067e-C = 1.008-C = 2.975e-C = 1.389e-C = 2.502e-C = 0.00 = 34 = 1.110421e = 5.587726e of species Activity 3.687e-006 2.691e-009 9.911e-001 0.000e+000 1.200e-001 1.435e-002	Charge Adjust 000 002 001 14 +002 +001 Log Molality -5.321 -8.383 1.744 -141.384 -0.961 -1.691	E balance ed to redox Iog Activity -5.433 -8.570 -0.004 -141.343 -0.921 -1.843
equilibrium Percent error Log Gamma -0.113 -0.187 0.000 C(-4) 0.041 C(4) 0.041 -0.152 0.052	Activ Ir Mass of Total alkali Total	pH pe rity of water mic strength fowater (kg) mity (eq/kg) (C2 (ml/kg) http: (C2 (ml/kg) http: (C2 (ml/kg) for a (kg) for	= 5.433 = 15.169 = 0.991 = 4.067e-C = 1.389e-C = 2.975e-C = 2.975e-C = 0.00 = 34 0.00 = 34 Activity 3.687e-006 2.691e-009 9.911e-001 0.000e+000 1.200e-001 1.435e-002 6.407e-003	Charge Adjust 001 002 001 114 ++002 ++001 	E balance ed to redox Log Activity -5.433 -8.570 -0.004 -141.343 -0.921 -1.843 -2.193
equilibrium Percent error Log Gamma -0.113 -0.187 0.000 C(-4) 0.041 C(4) 0.041 -0.152 -0.152 -0.152	Activ Ir Mass of Total alkali Tempera Electrical or, 100*(Cat- An  Cat- Species H+ CH- H2O 0.000e+000 CH4 1.389e-001 CC2 HCO3- CaHCO3+ MgHCO3+	pH pe rity of water mic strength for water (kg) mity (eq/kg) (C2 (ml/kg) htrze (cag (C) (C2 (ml/kg) htrze (cag (C) (C2 (ml/kg) ntratice Total H Total O Distribution of Molality 4.778e-006 4.143e-009 5.551e+001 0.000e+000 1.093e-001 2.039e-002 9.101e-003 5.771e-005	= 5.433 = 15.169 = 0.991 = 4.067e-C = 1.389e-C = 2.975e-C = 2.975e-C = 0.00 = 34 0.00 = 0.00 = 0.	Charge Adjust 001 002 001 114 ++002 ++001 Tog Molality -5.321 -8.383 1.744 -141.384 -0.961 -1.691 -2.041 -4.239	E balance ed to redox Log Activity -5.433 -8.570 -0.004 -141.343 -0.921 -1.843 -2.193 -4.375
equilibrium Percent error Log Gamma -0.113 -0.187 0.000 C(-4) 0.041 C(4) 0.041 -0.152 -0.152 -0.152 -0.136 0.0152	Activ Ir Mass of Total alkali Tempera Electrical or, 100*(Cat- An  Cat- Species H+ CH- H2O 0.0000e+000 CH4 1.389e-001 C02 HC03- CatC03+ MgHC03+ Fe_diHC03+	pH pe rity of water mic strength fwater (kg) mity (ed/kg) (C2 (ml/kg) hinre (cag ) (C2 training trans (cag ) (Cat+[An]) Iterations Total 0 Distribution of Molality 4.778e-006 4.143e-009 5.551e+001 0.000e+000 1.093e-001 2.039e-002 9.101e-003 5.771e-005 2.653e-005	= 5.433 = 15.169 = 0.991 = 4.067e-C = 1.2087e-C = 1.2087e-C = 1.2087e-C = 1.2087e-C = 1.2087e-C = 2.502e-C = 34 0.00 = 34 0.00 = 34 0.00 = 34 0.00 = 34 0.00 = 34 0.00 = 4.002 = 5.587726e 0.0 = 34 0.002 = 0.00 = 34 0.002 = 0.00 = 34 0.002 = 0.00 = 34 0.002 = 0.00 = 34 0.002 = 0.00 = 0.00 = 0.002 = 0.002	Charge Adjust 001 002 001 114 ++002 ++001 Molality -5.321 -8.383 1.744 -141.384 -0.961 -1.691 -2.041 -4.239 -4.576	Log Activity -5.433 -8.570 -0.004 -141.343 -0.921 -1.843 -2.193 -4.375 -4.712
equilibrium Percent error Log Gamma -0.113 -0.187 0.000 C(-4) 0.041 C(4) 0.041 -0.152 -0.152 -0.152 -0.136 -0.136 -0.136	Activ Iso Total alkalia Total Tot	pH pe rity of water nic strength for water (kg) inity (eg/kg) (C2 (mol/kg) three (cdg C) )/ (Cat+lAn]) Iterations Total O Distribution of Molality 4.778e-006 4.143e-009 5.551e+001 0.000e+000 1.093e-001 2.039e-002 9.101e-003 5.771e-005 2.653e-005 9.770e-006	= 5.433 = 15.169 = 0.991 = 4.067e-0 = 1.000e-0 = 2.975e-0 = 2.500 = 2.500 = 2.500 = 34 = 1.11042te = 5.587726e of species Activity 3.687e-006 2.691e-009 9.911e-001 1.435e-002 6.407e-003 4.218e-005 1.939e-005 1.073e-005	Charge Adjust 001 002 001 114 ++002 ++001 Molality -5.321 -8.383 1.744 -141.384 -0.961 -1.691 -2.041 -4.239 -4.576 -5.010	Log Activity -5.433 -8.570 -0.004 -141.343 -0.921 -1.843 -2.193 -4.375 -4.712 -4.969
equilibrium Percent error  Log Gamma -0.113 -0.187 0.000 C(-4) 0.041 C(4) 0.041 -0.152 -0.152 -0.152 -0.136 -0.136 0.041 0.041 -0.152	Activ Iso Total alkali Total Tota	pH pe ricy of water nic strength fwater (kg) nity (cg/kg) thre (cg) plance (cg) )/(Cat+lAn) Iterations Total H Total O Distribution of A.143e-009 5.551e+001 0.000e+000 1.093e-001 2.039e-002 9.101e-003 5.771e-005 2.653e-005 9.770e-006 2.168e-006	= 5.433 = 15.169 = 0.991 = 4.067e-0 = 1.000e-0 = 2.975e-0 = 2.500 = 2.500 = 2.500 = 34 = 1.110242 = 5.587726e of species Activity 3.687e-006 2.691e-009 9.911e-001 1.435e-002 6.407e-003 4.218e-005 1.939e-005 1.073e-005 2.381e-006	Charge Adjust 001 002 001 114 ++002 ++001 Molality -5.321 -8.383 1.744 -141.384 -0.961 -1.691 -2.041 -4.239 -4.576 -5.010 -5.664	Log Activity -5.433 -8.570 -0.004 -141.343 -0.921 -1.843 -2.193 -4.375 -4.712 -4.969 -5.623
equilibrium Percent error  Log Gamma -0.113 -0.187 0.000 C(-4) 0.041 -0.152 -0.152 -0.152 -0.136 0.041 0.041 0.041 0.041 -0.152 -0.136 0.041 0.04	Activ Mass of Total alkali Total Tot	pH pe ricy of water nic strength fowater (kg) nity (cg/kg) (C2 (ml/kg) (C2 (ml	= 5.433 = 15.169 = 0.991 = 4.067e-0 = 1.000e-0 = 2.975e-0 = 2.502e-0 = 0.00 = 2.502e-0 = 1.11042a = 5.587726e of species Activity 3.687e-006 2.691e-009 9.911e-001 1.435e-002 6.407e-003 4.218e-005 1.939e-005 1.073e-005 2.381e-006 1.826e-007	Charge Adjust 001 002 001 114 ++002 ++001 Molality -5.321 -8.383 1.744 -141.384 -0.961 -1.691 -2.041 -4.239 -4.576 -5.010 -5.664 -6.129	Log Activity -5.433 -8.570 -0.004 -141.343 -0.921 -1.843 -2.193 -4.375 -4.712 -4.969 -5.623 -6.739
equilibrium Percent error  Log Gamma -0.113 -0.187 0.000 C(-4) 0.041 -0.152 -0.152 -0.152 -0.136 -0.136 0.041 0.041 0.041 -0.152 -0.136 0.041 0.041 0.041 -0.152	Activ Mass of Total alkali Total Tot	pH pe ricy of water nic strength fwater (kg) nity (cg/kg) (C2 (ml/kg) (C2 (ml/	= 5.433 = 15.169 = 0.991 = 4.067e-0 = 1.000e-0 = 2.975e-0 = 2.502e-0 = 0.00 = 2.502e-0 = 1.11042 = 5.587726e of species Activity 3.687e-006 2.691e-009 9.911e-001 1.200e-001 1.435e-002 6.407e-003 4.218e-005 1.939e-005 1.939e-005 1.939e-005 1.826e-007 7.572e-008	Charge Adjust 001 002 001 114 ++002 ++001 Molality -5.321 -8.383 1.744 -141.384 -0.961 -1.691 -2.041 -4.239 -4.576 -5.010 -5.664 -6.129 -6.985	Log Activity -5.433 -8.570 -0.004 -141.343 -0.921 -1.843 -2.193 -4.375 -4.712 -4.969 -5.623 -6.739 -7.121
equilibrium Percent error  Log Gamma -0.113 -0.187 0.000 C(-4) 0.041 -0.152 -0.152 -0.152 -0.136 0.041 0.041 0.041 -0.152 -0.136 0.041 0.041 -0.136	Activ Mass of Total alkali Total Tot	pH pe ricy of water nic strength for water (kg) nity (cg/kg) (C2 (ml/kg) (C2 (	= 5.433 = 15.169 = 0.991 = 4.067e-0 = 1.000e-0 = 2.975e-0 = 2.502-0 = 0.00 = 2.502-0 = 0.00 = 2.502-0 = 0.00 = 2.502-0 = 1.11042 = 5.587726c of species	Charge Adjust 001 000 002 001 114 +002 +0001 	Log Activity -5.433 -8.570 -0.004 -141.343 -0.921 -1.843 -2.193 -4.375 -4.712 -4.969 -5.623 -6.739 -7.121 -7.228
equilibrium Percent error Camma  Log Gamma -0.113 -0.187 0.000 C(-4) 0.041 -0.152 -0.152 -0.136 -0.136 0.041 -0.610 -0.136 0.041 0.041	Activ Mass of Total alkali Total Total Total Total Tempera Electrical or, 100*(Cat- An  Cat: Species H+ CH- H2O 0.0000e+000 CH4 1.339e-001 CO2 HCO3- Cat: Cat: Cat: Cat: Cat: Cat: Cat: Cat:	pH pe ricy of water nic strength fwater (kg) nity (cg/kg) (C2 (ml/kg) (C2 (ml/	= 5.433 = 15.169 = 0.991 = 4.067e-0 = 1.000e-0 = 2.975e-0 = 2.502e-0 = 0.00 = 2.502e-0 = 1.11042a = 5.587726e of species Activity 3.687e-006 2.691e-009 9.911e-001 1.200e-001 1.435e-002 6.407e-003 4.218e-005 1.939e-005 1.073e-005 2.381e-006 1.826e-007 7.572e-008 5.916e-008 4.375e-008	Charge Adjust 001 000 002 001 114 +002 +0001 	Log Activity -5.433 -8.570 -0.004 -141.343 -0.921 -1.843 -2.193 -4.375 -4.712 -4.969 -5.623 -6.739 -7.121 -7.228 -7.359

Nacco3- 1.372e-009 1.003e-009 -8.863 -8.999

-0.136

0.041	MinCO3	7.816e-010	8.584e-010	-9.107	-9.066
0.041 Ca	1.476e-001				
-0.568	Ca+2	1.293e-001	3.499e-002	-0.888	-1.456
0.041	Ca904	9.215e-003	1.012e-002	-2.036	-1.995
-0.152	CaHCO3+	9.101e-003	6.407e-003	-2.041	-2.193
0.041	CaCO3	9.770e-006	1.073e-005	-5.010	-4.969
-0.136	CaHSO4+	2.991e-007	2.186e-007	-6.524	-6.660
-0.136	CaCH+	2.136e-009	1.561e-009	-8.670	-8.807
cl	2.367e-001	2 367e-001	1 559-001	-0.626	-0.807
-0.181	Te dicl+	3 978-006	2 907-006	-5.400	_5 537
-0.136	MpC]+	5 1440 009	3 7590 000	7 290	7 /25
-0.136	Eo triCl+2	5 9290 009	1 6920 000	9 227	0.777
-0.545	re_unut+z	0.329e-009	1.092e-009	-0.227	-0.772
0.041	MILLZ	2.3290-009	2.5580-009	-8.000	-8.392
-0.136	Fe_tricl2+	1.612e-009	1.1/8e-009	-8.793	-8.929
-0.136	MnCL3-	1.503e-010	1.098e-010	-9.823	-9.959
0.041	Fe_triCL3	1.672e-011	1.836e-011	-10.777	-10.736
Fe_di	8.109e-005 Fe_di+2	4.735e-005	1.351e-005	-4.325	-4.869
-0.545	Fe_diH003+	2.653e-005	1.939e-005	-4.576	-4.712
-0.136	Fe diCl+	3.978e-006	2.907e-006	-5.400	-5.537
-0.136	Fe diSO4	3.171e-006	3.482e-006	-5.499	-5.458
0.041	Fe di(0)3	5.387e-008	5.916e-008	-7.269	-7.228
0.041	Fe diOH+	1 571-009	1 1/18-009	_8 804	_8 9/0
-0.136	Fe ditant	1 155-010	8 ///0=_011	_9 937	_10_074
-0.136	Fe di (HS)?	0.000e+000	0.000+000	_274_815	_274 774
0.041	Te_di (IIC)2	0.000=:000	0.000-000	412 020	110 164
-0.136	re_ut(h5)5-	0.00000000	0.00000000	-412.020	-412.104
re_tri	7.991e-005 Fe_tri (OH) 2+	7.595e-005	5.551e-005	-4.119	-4.256
-0.136	Fe_triOH+2	2.186e-006	6.236e-007	-5.660	-6.205
-0.545	Fe_tri(OH)3	1.750e-006	1.922e-006	-5.757	-5.716
0.041	Fe_triSO4+	7.814e-009	5.711e-009	-8.107	-8.243
-0.136	Fe_tri+3	6.041e-009	3.593e-010	-8.219	-9.445
-1.226	Fe_triCl+2	5.929e-009	1.692e-009	-8.227	-8.772
-0.545	Fe_triCl2+	1.612e-009	1.178e-009	-8.793	-8.929
-0.136	Fe_tri2(OH)2+4	1.580e-009	1.047e-011	-8.801	-10.980
-2.179	Fe tri(OH)4-	6.448e-010	4.713e-010	-9.191	-9.327
-0.136	Fe tri3(0H)4+5	3.081e-010	1.214e-013	-9.511	-12,916
-3.405	Fe tri (904)2-	2.478e-010	1.811e-010	-9.606	-9.742
-0.136	Fe triCl3	1 672-011	1 8360-011	_10 777	_10_736
0.041	Fo trill9042	1 9760 013	5 6390 014	12 704	13 2/0
-0.545	0.00000000	1.9708-015	5.0598-014	-12.704	-13.245
n(0)	H2	0.000e+000	0.000e+000	-44.396	-44.355
0.041 K	5.270e-005	5 000 005	2 440 005	4 000	4.400
-0.181	K+	5.222e-005	3.4400-005	-4.282	-4.463
-0.136	K904-	4.794e-007	3.5030-007	-6.319	-6.456
0.041	KOH	2.919e-014	3.206e-014	-13.535	-13.494
Mg	9.719e-004 Mg+2	8.364e-004	2.511e-004	-3.078	-3.600
-0.523	Mg904	7.772e-005	8.535e-005	-4.109	-4.069
0.041	MgHCO3+	5.771e-005	4.218e-005	-4.239	-4.375
-0.136	MpCO3	3.984e-008	4.375e-008	-7.400	-7.359
0.041	MpCH+	3.354e-010	2.451e-010	-9.474	-9.611
-0.136 Mn(2)	3.951e-007				
-0.576	Mn+2	2.229e-007	5.919e-008	-6.652	-7.228
-0.136	MnHCO3+	1.036e-007	7.572e-008	-6.985	-7.121
_0 136	MnCl+	5.144e-008	3.759e-008	-7.289	-7.425
0.041	MnSO4	1.390e-008	1.526e-008	-7.857	-7.816
0.041	MnCl2	2.329e-009	2.558e-009	-8.633	-8.592
0.041	Mn003	7.816e-010	8.584e-010	-9.107	-9.066
0.120	MnCl3-	1.503e-010	1.098e-010	-9.823	-9.959
-0.136	MnOH+	5.596e-013	4.090e-013	-12.252	-12.388
-∪.⊥36 Man(3)	4.541e-017				
-1.226	Min+3	4.541e-017	2.701e-018	-16.343	-17.568

Na	4.183e-004	1 132-001	2 951-001	_3 384	_3 530
-0.146	NECO	2 0220 004	2.1440.005	E E22	5.550
-0.136	14204-	2.5558-000	2.1446-000	-5.555	-5.005
0.041	Nahoos	2.1080-000	2.3810-000	-5.004	-5.023
-0.136	NaLO3-	1.3/2e-009	1.003e-009	-8.863	-8.999
0.041	NaCH	4.7/2e-013	5.240e-013	-12.321	-12.281
O(0)	3.828e-004 02	1.914e-004	2.102e-004	-3.718	-3.677
0.041 S(-2)	0.000e+000				
0.041	H2S	0.000e+000	0.000e+000	-137.960	-137.919
-0.187	HS-	0.000e+000	0.000e+000	-139.240	-139.427
-0.635	S-2	0.000e+000	0.000e+000	-146.277	-146.912
0.041	Fe_di(HS)2	0.000e+000	0.000e+000	-274.815	-274.774
0.126	Fe_di(HS)3-	0.000e+000	0.000e+000	-412.028	-412.164
S(6)	1.579e-002	0.215-0.02	1 012- 002	2 026	1 005
0.041	Ca304	9.2150-003	1.0120-002	-2.050	-1.990
-0.651	504-2	6.490e-003	1.4508-005	-2.188	-2.839
0.041	MgSO4	7.772e-005	8.535e-005	-4.109	-4.069
0.041	Fe_diS04	3.171e-006	3.482e-006	-5.499	-5.458
-0.136	NaSO4-	2.933e-006	2.144e-006	-5.533	-5.669
-0.136	H904-	7.110e-007	5.196e-007	-6.148	-6.284
-0.136	K904-	4.794e-007	3.503e-007	-6.319	-6.456
-0.136	CaHSO4+	2.991e-007	2.186e-007	-6.524	-6.660
0.041	MnSO4	1.390e-008	1.526e-008	-7.857	-7.816
0.120	Fe_triSO4+	7.814e-009	5.711e-009	-8.107	-8.243
-0.136	Fe_tri(SO4)2-	2.478e-010	1.811e-010	-9.606	-9.742
-0.136	Fe <u>diH</u> 904+	1.155e-010	8.440e-011	-9.937	-10.074
-0.136	Fe_triH904+2	1.976e-013	5.639e-014	-12.704	-13.249
-0.545					
		-Saturation i	ndices		
	Phase	SI log I	AP log KT		

Phase	SI log I	AP log KT	
Arbage Arbagenite Calcite Calcite C44(g) C02(g) Dolomite Cypsum H20(g) H	51 100 1 0.07 -4. 0.29 -8. -138.48 -141. 0.55 -0. -1.44 -188. 0.28 -8. -41.21 -44. -41.21 -44. -1.51 -0. -1.36.92 -137. -5.92 -4. -8.92 -52. -1.11 24. -0.79 -3. 3.46 44. -2.84 -13.	$\begin{array}{rrrrr} & -100 & \mathrm{K}^{-1} \\ 29 & -4.36 \\ 19 & -8.34 \\ 19 & -8.48 \\ 34 & -2.86 \\ 92 & -1.47 \\ 53 & -17.09 \\ 30 & -4.58 \\ 63 & -3.15 \\ 36 & -3.15 \\ 30 & 1.51 \\ 92 & -1.00 \\ 34 & 1.58 \\ 11 & 61.03 \\ 23 & 25.34 \\ 68 & -2.89 \\ 63 & 15.20 \\ 63 & 15.20 \\ 84 & 41.38 \\ 97 & -11.13 \end{array}$	CaSO4 CaCO3 CaCO3 Cf4 Cf2 CaSO4:2:H2O H2O H2O H2O H2O H2O MaCL MaOCH O2 MaOCH O2 MaCO3 MaCO3 MaCO3
Sulfur	-101.60 -96.	71 4.88	S

Reaction step 5.

Na

Using solution 1. Using pure phase assemblage 1. Using kinetics 1. Kinetics defined in simulation 2. Kinetics 1. Kinetics defined in simulation 2.

Coefficient	Rate name	Delta Moles Total Mole	s Reactant
1	Fe <u>di</u> ax	-5.198e-005 9.999e-00	1 Fe_di
-1			Fe_tri
		Phase assemblage	
			Moles in assemblage

Delta		Phase	SI	log IAP	log KT	Initial	Final
	1.300e-005	02 (g)	-0.78	-3.68	-2.89	1.000e+001	1.000e+001-
			Solution	ı canposi	tion		

Elements	Molality	Moles
C Ca Cl Fe_Cii Fe_tri K Mg Mn Ma	1.389e-001 1.476e-001 2.367e-001 2.911e-005 1.319e-005 9.719e-004 3.951e-007 4.183e-004	1.389e-001 1.476e-001 2.367e-001 2.911e-005 1.319e-004 5.270e-005 9.719e-004 3.951e-007 4.183e-004

	S	1.579e-002	1.579e-002		
	D	escription of	solution		
		pH	= 5.433	Charge	balance
equilibrium Percent err	Activ Ic Mass c Total alkali Total Tempera Electrical or, 100*(Cat- An	pe rity of water nic strength f water (kg) nity (eg/kg) CO2 (mol/kg) ture (deg C) balance (eg) )/(Cat+ An ) Iterations Total H Total O	= 15.170 = 0.991 = 4.067e-C = 1.000e+C = 2.980e-C = 1.389e-C = 25.000 = 2.537e-C = 0.00 = 85 = 1.110421e = 5.587729e	Adjust 101 100 102 101 114 \$+002 \$+001	ed to redax
	T	istribution c	f species		
Log				Log	Log
Gamma	Species	Molality	Activity	Molality	Activity
	H+	4.786e-006	3.693e-006	-5.320	-5.433
-0.113	OH-	4.137e-009	2.687e-009	-8.383	-8.571
-0.187	H2O	5 551e+001	9 911-001	1 744	-0.004
0.000	0.000+000	5.55101001	J.JIIC 001	1./11	0.001
0.041	CH4	0.000e+000	0.000e+000	-141.384	-141.343
0.0/1	02	1.094e-001	1.201e-001	-0.961	-0.920
-0 152	HCO3-	2.036e-002	1.434e-002	-1.691	-1.844
0.150	CaHCO3+	9.090e-003	6.399e-003	-2.041	-2.194
0.120	MgHCO3+	5.765e-005	4.213e-005	-4.239	-4.375
-0.136	CaCO3	9.743e-006	1.070e-005	-5.011	-4.971
0.041	Fe_diHCO3+	9.515e-006	6.954e-006	-5.022	-5.158
-0.136	NaHCO3	2.166e-006	2.379e-006	-5.664	-5.624
0.041	003-2	7.412e-007	1.820e-007	-6.130	-6.740
-0.610	MnHCO3+	1.035e-007	7.565e-008	-6.985	-7.121
-0.136	MgCO3	3.973e-008	4.363e-008	-7.401	-7.360
0.041	Fe_diC03	1.929e-008	2.118e-008	-7.715	-7.674
0.041	NaCO3-	1.369e-009	1.000e-009	-8.864	-9.000
-0.136	MinCO3	7.797e-010	8.562e-010	-9.108	-9.067
0.041 Ca	1.476e-001	1 293-001	3 499-002	-0.888	-1 456
-0.568	Ca904	9 216-003	1 012-002	-2 035	_1 995
0.041	C=1003+	9 0905 003	6 3000 003	2.000	2 104
-0.152	Cances+	9.0908-005	1 070- 005	-2.041	-2.134
0.041	Calus	9.745e-006	1.070e-005	-5.011	-4.9/1
-0.136	CaHSO4+	2.9966-007	2.1908-007	-6.523	-6.660
-0.136 Cl	2.367e-001	2.1328-009	1.5580-009	-8.6/1	-8.807
-0.181	CI-	2.367e-001	1.559e-001	-0.626	-0.807
-0.136	re <u>d</u> iCl+	1.428e-006	1.044e-006	-5.845	-5.981
-0.136	MnC1+	5.146e-008	3.761e-008	-7.289	-7.425
-0.545	re_triCl+2	9.818e-009	2.801e-009	-8.008	-8.553
-0.136	re_triCl2+	2.669e-009	1.950e-009	-8.574	-8.710
0.041	MhCL2	2.330e-009	2.559e-009	-8.633	-8.592
-0.136	MnCL3-	1.504e-010	1.099e-010	-9.823	-9.959
0.041 Fe_di	Fe_triCl3 2.911e-005	2.769e-011	3.041e-011	-10.558	-10.517
-0.545	Fe_di+2	1.700e-005	4.851e-006	-4.769	-5.314
-0.136	Fe_diHCO3+	9.515e-006	6.954e-006	-5.022	-5.158
-0.136	Fe_diCl+	1.428e-006	1.044e-006	-5.845	-5.981
0.041	Fe_diSO4	1.139e-006	1.251e-006	-5.944	-5.903
0.041	Fe_diCO3	1.929e-008	2.118e-008	-7.715	-7.674
-0.136	Fe_diOH+	5.633e-010	4.117e-010	-9.249	-9.385
-0.136	Fe_diH904+	4.154e-011	3.036e-011	-10.382	-10.518
0.041	Fe_di(HS)2	0.000e+000	0.000e+000	-275.258	-275.217
-0.136	Fe <u>di</u> (HS)3-	0.000e+000	0.000e+000	-412.471	-412.607
Fe_tri -0.136	1.319e-004 Fe_tri(OH)2+	1.253e-004	9.161e-005	-3.902	-4.038
-0.545	Fe_tri0H+2	3.614e-006	1.031e-006	-5.442	-5.987

	Fe_tri(OH)3	2.884e-006	3.167e-006	-5.540	-5.499
0.041	Fe_triSO4+	1.294e-008	9.457e-009	-7.888	-8.024
-0.136	Fe_tri+3	1.000e-008	5.949e-010	-8.000	-9.226
-1.226	Fe triCl+2	9.818e-009	2.801e-009	-8.008	-8.553
-0.545		4.318e-009	2.860e-011	-8.365	-10.544
-2.179	Fe triCl2+	2.669e-009	1.950e-009	-8.574	-8.710
-0.136	Fe tri3(0H)/4+5	1 390-009	5 /7/0-013	_8 .857	_12 262
-3.405	Te_cris(CI)4+5	1.061-000	7 7520 010	0.007/	0 111
-0.136	Fe_tri (GO() 2	1.0010-009	7.7528-010	-0.9/4	-9.111
-0.136	Fe_tr1(504)2-	4.1040-010	3.000e-010	-9.387	-9.523
0.041	Fe_trici3	2.769e-011	3.0410-011	-10.558	-10.517
-0.545 H(0)	Fe_triH904+2 0.000e+000	3.2/8e-013	9.353e-014	-12.484	-13.029
0.041 K	H2 5.270e-005	0.000e+000	0.000e+000	-44.396	-44.355
-0.181	K+	5.222e-005	3.440e-005	-4.282	-4.463
-0.136	K904-	4.794e-007	3.504e-007	-6.319	-6.455
0.041 Mg	КОН 9.719е-004	2.915e-014	3.201e-014	-13.535	-13.495
-0.522	Mg+2	8.365e-004	2.512e-004	-3.078	-3.600
0.041	Mg904	7.773e-005	8.536e-005	-4.109	-4.069
_0 136	MgHCO3+	5.765e-005	4.213e-005	-4.239	-4.375
0.041	MgCO3	3.973e-008	4.363e-008	-7.401	-7.360
0.120	MgCH+	3.349e-010	2.447e-010	-9.475	-9.611
-0.136 Mn(2)	3.951e-007	2 230-007	5 921-008	-6 652	_7 228
-0.576	Melinia.	1 0350 007	7 5650 000	6 995	7 121
-0.136	MIRLOST	E 14C- 000	7.3050-000	-0.905	-7.121
-0.136	MICI+	1 200 000	1.507.000	-7.209	-7.423
0.041	Mn304	1.390e-008	1.52/e-008	-/.85/	-7.816
0.041	MnC12	2.330e-009	2.559e-009	-8.633	-8.592
0.041	MhCO3	'/.'/9/e-010	8.562e-010	-9.108	-9.067
-0.136	MnCl3-	1.504e-010	1.099e-010	-9.823	-9.959
-0.136	MnCH+	5.589e-013	4.085e-013	-12.253	-12.389
Mn(3) -1.226	4.550e-017 Mn+3	4.550e-017	2.707e-018	-16.342	-17.568
Na	4.183e-004 Na+	4.132e-004	2.951e-004	-3.384	-3.530
-0.146	NaSO4-	2.933e-006	2.144e-006	-5.533	-5.669
-0.136	NaHCO3	2.166e-006	2.379e-006	-5.664	-5.624
0.041	NB(103-	1 369-009	1 000-009	-8 864	-9.000
-0.136	NHON	4 7640 013	5 2320 013	12 322	12 201
0.041 O(0)	3.828e-004	1 91/0-00/	2 102-004	_3 718	-3 677
0.041 S(-2)	0.000e+000	0.000~+000	0.000-+000	137 059	137 019
0.041	120	0.000-000	0.000-000	120.000	120 427
-0.187	10- 10-	0.000000	0.000000	146 000	146 010
-0.635	5-2	0.000000000	0.0000+000	-140.277	-140.912
0.041	Fe_d1 (HS) 2	0.000e+000	0.000e+000	-2/5.258	-2/5.21/
-0.136 S(6)	Fe_d1 (HS) 3- 1.579e-002	0.000e+000	0.000e+000	-412.471	-412.607
0.041	Ca504	9.216e-003	1.012e-002	-2.035	-1.995
-0.651	SO4-2	6.490e-003	1.450e-003	-2.188	-2.839
0.041	Mg904	7.773e-005	8.536e-005	-4.109	-4.069
-0.136	Na904-	2.933e-006	2.144e-006	-5.533	-5.669
0.041	Fe_diSO4	1.139e-006	1.251e-006	-5.944	-5.903
-0.136	HSO4-	7.123e-007	5.206e-007	-6.147	-6.284
-0.136	K904-	4.794e-007	3.504e-007	-6.319	-6.455
_0 136	CaHSO4+	2.996e-007	2.190e-007	-6.523	-6.660
0.041	MnSO4	1.390e-008	1.527e-008	-7.857	-7.816
0.120	Fe_triSO4+	1.294e-008	9.457e-009	-7.888	-8.024
-0.130	Fe_tri(SO4)2-	4.104e-010	3.000e-010	-9.387	-9.523
-0.136	Fe_diH904+	4.154e-011	3.036e-011	-10.382	-10.518
-0.136	Fe_triH904+2	3.278e-013	9.353e-014	-12.484	-13.029
-0.545					
		-Saturation i	ndices		

Phase	SI	log IAP	log KT	
Anhydrite	0.07	-4.29	-4.36	Ca904
Aragonite	0.14	-8.20	-8.34	CaCO3
Calcite	0.28	-8.20	-8.48	CaCO3
CH4 (q)	-138.48	-141.34	-2.86	CH4
CC2 (g)	0.55	-0.92	-1.47	CC2
Dolomite	-1.45	-18.54	-17.09	CaMg(003)2
Gypsum	0.28	-4.30	-4.58	Ca904:2H20
H2 (g)	-41.21	-44.36	-3.15	H2
H2O(g)	-1.51	-0.00	1.51	H2O
H2S(g)	-136.92	-137.92	-1.00	H2S
Halite	-5.92	-4.34	1.58	NaCl
Hausmannite	-8.93	52.10	61.03	Mn304
Manganite	-1.11	24.23	25.34	MinOOH
02 (g)	-0.78	-3.68	-2.89	02
Pyrochroite	-11.57	3.63	15.20	Min (OH) 2
Pyrolusite	3.46	44.84	41.38	MinO2
Rhodochrosite	-2.84	-13.97	-11.13	MinCO3
Sulfur	-101.59	-96.71	4.88	S

Reaction step 6.

-0.136

0.041

CaCO3

WARNING: Element Fe di has negative moles in solution, -4.123295e-006. Erroneous mole balance occurs as moles are added to produce zero moles. Usually caused by KINETICS, REACTION, or diffuse layer calculation. calculation. May be due to large time steps in early part of KINETICS simulation or negative concentrations in the diffuse layer. Using solution 1. Using purphase assemblage 1. Using kinetics 1. Kinetics defined in simulation 2. Kinetics 1. Kinetics defined in simulation 2. Time step: 50400 seconds (Incremented time: 86400 seconds) Delta Moles Total Moles Reactant Rate name Coefficient Fe\_di\_ax -2.642e-005 9.998e-001 Fe\_di -1 Fe\_tri 1 -Phase assemblage-Moles in assemblage SI log IAP log KT Initial Final Phase Delta 02 (g) -0.78 -3.68 -2.89 1.000e+001 1.000e+001-6.607e-006 -Solution composition---Elements Molality Moles 
 1.389e-001
 1.389e-001

 1.476e-001
 1.476e-001

 2.367e-001
 2.367e-001

 2.681e-005
 2.681e-006

 1.583e-004
 1.583e-004

 5.270e-005
 5.270e-005

 9.719e-004
 9.719e-004

 3.951e-007
 4.138e-004

 4.138e-004
 4.138e-004

 5.70e-005
 2.578e-002
 C Ca Cl Fe\_di Fe\_tri K Mg Ma Na S -Description of solutionpH = 5.432 pe = 15.170 Charge balance Adjusted to redox equilibrium equilibrium Activity of water = Ionic strength = Mass of water (kg) = Total alkalinity (eg/kg) = Total (CO2 (mol/kg) = Tamperature (kg C) = Electrical balance (eg) = Percent error, 100\*(Cat-[An])/(Cat+[An]) = Terations = 0.991  $\begin{array}{rcl} = & 0.991 \\ = & 4.066e-001 \\ = & 1.000e+000 \\ = & 2.983e-002 \\ = & 1.389e-001 \\ = & 25.000 \\ = & 1.721e-013 \\ = & 0.00 \\ = & 85 \\ = & 1.110(21e+0) \end{array}$ Total H = 1.110421e+002 Total 0 = 5.587730e+001 -Distribution of species-Log Log Log Species Molality Activity Molality Activity Gamma H+ 4.790e-006 3.696e-006 -5.320 -5.432 -0.113 OH-4.133e-009 2.684e-009 -8.384 -8.571 -0.187 H2O 5.551e+001 9.911e-001 1.744 -0.004 0.000 C(-4) 0.000e+000 CH4 0.000e+000 0.000e+000 -141.384 -141.343 0.041 C(4) 1.389e-001 002 -0.961 1.094e-001 1.201e-001 -0.920 0.041 HCO3-2.035e-002 1.433e-002 -1.691 -1.844 -0.152 CaHCO3+ 9.085e-003 6.396e-003 -2.042 -2.194 -0.152 MgHCO3+ 5.761e-005 4.211e-005 -4.239 -4.376

9.730e-006 1.068e-005

-5.012

-4.971

0.041	NaHCO3	2.165e-006	2.377e-006	-5.665	-5.624
0.041	Fe_diH003+	8.762e-007	6.403e-007	-6.057	-6.194
-0.130	003-2	7.401e-007	1.818e-007	-6.131	-6.740
-0.010	MinHCO3+	1.035e-007	7.562e-008	-6.985	-7.121
-0.130	MgCO3	3.967e-008	4.357e-008	-7.401	-7.361
0.041	Fe_diC03	1.775e-009	1.949e-009	-8.751	-8.710
0.041	NaCO3-	1.367e-009	9.987e-010	-8.864	-9.001
-0.130	MinCO3	7.787e-010	8.551e-010	-9.109	-9.068
Ca	1.476e-001	1 202- 001	2 400- 002	0 000	1 /56
-0.568	Ca#2	0.217-002	1 012- 002	-0.000	-1.400
0.041	Callon	9.21/0-003	6 2060 002	2.035	2 104
-0.152	C-002	9.0000-005	1 060- 005	-2.042	-2.194
0.041	Callford	2,000-,007	2 102- 007	-5.012	-4.971
-0.136	Canso4+	2.3350-007	1 5570 000	-0.525	0.000
-0.136	0.207-001	2.1318-009	1.00/e-009	-0.0/2	-0.000
0.101	2.36/e-001 Cl-	2.367e-001	1.559e-001	-0.626	-0.807
-0.181	Fe_diCl+	1.316e-007	9.618e-008	-6.881	-7.017
-0.130	MnCl+	5.147e-008	3.761e-008	-7.288	-7.425
-0.136	Fe_triCl+2	1.180e-008	3.368e-009	-7.928	-8.473
-0.545	Fe_triCl2+	3.209e-009	2.345e-009	-8.494	-8.630
-0.136	MnCl2	2.331e-009	2.560e-009	-8.632	-8.592
0.041	MnCl3-	1.504e-010	1.099e-010	-9.823	-9.959
-0.136	Fe_triCl3	3.329e-011	3.656e-011	-10.478	-10.437
0.041 Fe_di	2.681e-006	1 5 67 000	4 470 007	5 005	6 250
-0.545	Fe <u>d</u> 1+2	1.56/e-006	4.4/0e-00/	-5.805	-6.350
-0.136	Fe <u>diHCU3</u> +	8.762e-007	6.403e-007	-6.057	-6.194
-0.136	Fe_diCl+	1.316e-007	9.618e-008	-6.881	-7.017
0.041	Fe_diS04	1.049e-007	1.152e-007	-6.979	-6.938
0.041	Fe <u>d</u> icus	1.7/5e-009	1.949e-009	-8.751	-8.710
-0.136	Fe_diOH+	5.186e-011	3.790e-011	-10.285	-10.421
-0.136	Fe_diH904+	3.831e-012	2.800e-012	-11.417	-11.553
0.041	Fe_di(HS)2	0.000e+000	0.000e+000	-2/6.293	-276.252
-0.136	Fe_d1 (HS) 3-	0.00000000	0.00000+000	-413.505	-413.641
Fe <u>t</u> ri	1.583e-004 Fe_tri(OH)2+	1.505e-004	1.100e-004	-3.823	-3.959
-0.136	Fe_triOH+2	4.341e-006	1.238e-006	-5.362	-5.907
-0.545	Fe_tri(OH)3	3.459e-006	3.798e-006	-5.461	-5.420
0.041	Fe <u>tri</u> 904+	1.556e-008	1.137e-008	-7.808	-7.944
-0.136	Fe_tri+3	1.203e-008	7.153e-010	-7.920	-9.146
-1.226	Fe_triCl+2	1.180e-008	3.368e-009	-7.928	-8.473
-0.545	Fe_tri2(OH)2+4	6.232e-009	4.128e-011	-8.205	-10.384
-2.179	Fe_triCl2+	3.209e-009	2.345e-009	-8.494	-8.630
-0.136	Fe_tri3(OH)4+5	2.407e-009	9.483e-013	-8.619	-12.023
-3.405	Fe_tri (OH) 4-	1.271e-009	9.289e-010	-8.896	-9.032
-0.136	Fe_tri(SO4)2-	4.935e-010	3.607e-010	-9.307	-9.443
-0.136	Fe_triCl3	3.329e-011	3.656e-011	-10.478	-10.437
0.041	Fe_triH904+2	3.945e-013	1.125e-013	-12.404	-12.949
-0.545 H(0)	0.000e+000				
0.041	H2	0.00000000	0.00000+000	-44.396	-44.355
K	5.2/0e-005 K+	5.222e-005	3.440e-005	-4.282	-4.463
-0.181	K904-	4.794e-007	3.504e-007	-6.319	-6.455
-0.130	KOH	2.912e-014	3.198e-014	-13.536	-13.495
0.041 Mg	9.719e-004	0.005 004	0 540 004	0.050	0.000
-0.522	Mg+2	8.365e-004	2.512e-004	-3.078	-3.600
0.041	143504	1.//4e-005	0.53/e-005	-4.109	-4.069
0.120	D0000 F F 1 1 1 1	э./юте-002	4.211e-005	-4.239	-4.576
-0.130	MgHLUS+	2.007 000	4 357 000	7 404	7 200
0.041	MgHLO3+ MgCO3	3.967e-008	4.357e-008	-7.401	-7.361
-0.136 0.041 -0.136	MgCO3 MgCH+	3.967e-008 3.346e-010	4.357e-008 2.445e-010	-7.401 -9.475	-7.361 -9.612
-0.136 0.041 -0.136 Mn(2)	MgCO3 MgCH+ 3.951e-007 Mn+2	3.967e-008 3.346e-010 2.230e-007	4.357e-008 2.445e-010 5.922e-008	-7.401 -9.475 -6.652	-7.361 -9.612 -7.228
-0.136 0.041 -0.136 Mn(2) -0.576	MgHLOS+ MgCO3 MgCH+ 3.951e-007 Mn+2 MnHCO3+	3.967e-008 3.346e-010 2.230e-007 1.035e-007	4.357e-008 2.445e-010 5.922e-008 7.562e-008	-7.401 -9.475 -6.652 -6.985	-7.361 -9.612 -7.228 -7.121

0.405	MnCl+	5.147e-008	3.761e-008	-7.288	-7.425		
-0.136	Mn904	1.390e-008	1.527e-008	-7.857	-7.816		
0.041	MnC12	2.331e-009	2.560e-009	-8.632	-8.592		
0.041	MinCO3	7.787e-010	8.551e-010	-9.109	-9.068		
0.041	MnCl3-	1.504e-010	1.099e-010	-9.823	-9.959		
-0.136	MnCH+	5.585e-013	4.082e-013	-12.253	-12.389		
-0.136 Mn(3)	4.555e-017 Mn+3	4.555e-017	2.709e-018	-16.342	-17.567		
-1.226 Na	4.183e-004	4 122- 004	0.051004	2 204	3 530		
-0.146	Na+	4.132e-004	2.9510-004	-3.384	-3.530		
-0.136	N8904-	2.9340-006	2.1440-006	-5.533	-5.669		
0.041	NAHLUS	2.1658-006	2.3//e-006	-5.005	-5.624		
-0.136	Nacos-	1.36/e-009	9.98/e-010	-8.864	-9.001		
0.041 O(0)	3.828e-004	4.700e-013	2 102-004	-12.322	-12.282		
0.041	0.000e+000	1.9140 004	2.1020 004	5.710	5.077		
0.041	H2S	0.000e+000	0.000e+000	-137.957	-137.917		
_0 187	HS-	0.000e+000	0.000e+000	-139.239	-139.426		
-0.635	S-2	0.000e+000	0.000e+000	-146.277	-146.912		
-0.035	Fe_di(HS)2	0.000e+000	0.000e+000	-276.293	-276.252		
0.136	Fe_di(HS)3-	0.000e+000	0.000e+000	-413.505	-413.641		
-0.136 S(6)	1.579e-002	9 217e-003	1 012-002	-2 035	_1 995		
0.041	and 2	6 491o 003	1 4500 003	2.000	2 930		
-0.651	304-2 M=004	7 774- 005	2.430e-005	-2.100	-2.039		
0.041	149304 1597/	2 9340 006	2 1440 006	-4.109	-4.009		
-0.136	10004-	7 1290 007	5 2106 007	6 147	6 293		
-0.136	11304-	4 7040 007	2 5040 007	-0.147	-0.200		
-0.136	0-17004-	4.7940-007	3.304e-007	-0.319	-0.455		
-0.136	CaH504+	2.9998-007	2.192e-007	-6.523	-6.659		
0.041	re_diso4	1.0490-007	1.1520-007	-0.979	-0.938		
-0.136	Fe_tris04+	1.5568-008	1.13/e-008	-7.808	-7.944		
0.041	Mn904	1.3900-008	1.52/e-008	-7.857	-7.816		
-0.136	Fe_tr1 (504) 2-	4.935e-010	3.60/e-010	-9.307	-9.443		
-0.136	re_allhout+	3.851e-012	2.800e-012	-11.41/	-11.555		
-0.545	Fe_tr1H904+2	3.9450-013	1.1250-013	-12.404	-12.949		
		—Saturation i	ndices				
	Phase	SI log I	AP log KT				
Arhydrite         0.07         -4.29         -4.36         CaSDA           Aragonite         0.14         -8.20         -8.34         CaCDA           Calcite         0.28         -8.20         -8.48         CaCDA           CH4(g)         -138.48         -141.34         -2.86         CH4           CQ2(g)         0.55         -0.92         -1.47         CQ2           Dolarmite         -1.45         -18.54         -17.09         CaMg(CO3)2           Oppsam         0.28         -4.30         -4.58         CaSDA::EEO           H2(g)         -4.121         -44.36         -3.15         H2           H20(g)         -15.1         -0.00         1.51         H20           H2S(g)         -136.92         -137.92         -1.00         H21           Haistrem         -8.93         52.10         61.03         Mn3O4           Marganite         -8.93         52.10         61.03         Mn3O4           Marganite         -11.17         24.23         25.34         MnO2           Pyrolysite         3.45         44.83         41.38         MnO2           Rhadochrosite         -2.44         -13.97         -11.13         40.95<							
Reaction step	57.						
WARNING: Elen	rent Fe_di has ne	gative moles	in solution,	-5.710494	e-006.		
zero moles.	Erromeous mole balance occurs as moles are added to produce zero moles.						
calculation.	Usually caused by KINETICS, REACTION, or diffuse layer calculation.						
simulation or Using solutio Using pure pr Using kinetic	rnay be due to l r negative concer n 1. nase assemblage 1 ns 1. K	arge time ste itrations in t 1. inetics defin	ps in early he diffuse ] ed in simula	part of KI layer. tion 2.	NETICS		
Kinetics 1.	Kinetics define	d in simulati	an 2.				
	Time step: 8640	0 seconds (I	incremented t	time: 17280	0 seconds)		
Opeficiant	Rate name	Delta Moles	Total Moles	Reactant			

COEFFICIENC				
1	Fe_di_ox	-2.636e-006	9.998e-001	Fe_di
-1				Fe_tri
1				
		Phase asser	iblage	

Delta	Phase	SI log I	AP log KT	Moles in as Initial	semblage Fina
6.591e-007	C2 (g)	-0.79 -3.	68 -2.89	1.000e+001	1.000e+00
		-Solution comp	osition		
	Elements	Molality	Moles		
	C Ca Cl Fe_tri K Mg Mn Na S	1.389e-001 1.476e-001 2.367e-001 4.531e-008 1.610e-004 5.270e-005 9.719e-004 3.951e-007 4.183e-004 1.579e-002	1.389e-001 1.476e-001 2.367e-001 4.531e-008 1.610e-004 5.270e-005 9.719e-004 3.951e-007 4.183e-004 1.579e-002		
		Description of	solution		
equilibrium	Acti I Mass Total alkal Total Total	pH pe vity of water onic strength of water (kg) inity (eg/kg) .002 (mol/kg) ature (der C)	= 5.432 = 15.170 = 0.991 = 4.066e- = 1.000e+ = 2.983e- = 1.389e- = 25.000	Charge Adjust 001 000 002 001	e balance ted to red
Percent err	Electrical ar, 100*(Cat- An	balance (eg)  )/(Cat+ An ) Iterations Total H Total O	= 3.342e- = 0.00 = 92 = 1.110421 = 5.587731	013 e+002 e+001	
		Distribution o	f species		
Im				Log	Log
Gamma	Species	Molality	Activity	Molality	Activity
	H+	4.791e-006	3.697e-006	-5.320	-5.432
-0.113	OH-	4.133e-009	2.684e-009	-8.384	-8.571
0.000	H2O	5.551e+001	9.911e-001	1.744	-0.004
C(-4)	0.000e+000 CH4	0.000e+000	0.000e+000	-141.384	-141.34
0.0/1	1.389e-001 CC2	1.094e-001	1.201e-001	-0.961	-0.92
-0.152	H003-	2.035e-002	1.433e-002	-1.691	-1.84
-0.152	CaHCO3+	9.085e-003	6.396e-003	-2.042	-2.19
-0.136	MgHCO3+	5.761e-005	4.210e-005	-4.239	-4.376
0.041	CaCO3	9.729e-006	1.068e-005	-5.012	-4.97
0.041	Marillus marillus	2.1650-006	2.37/e-006	-5.665	-5.62
-0.610	MH1002+	1.035o.007	7 5620 008	-0.131	-0.74
-0.136	Marcos	3.967-008	4 356-008	-7 402	-7.36
0.041	Fe diHOO3+	1.481e-008	1.082e-008	-7.830	-7.96
-0.136	NaCO3-	1.366e-009	9,986e-010	-8.864	-9.00
-0.136	MhCO3	7.786e-010	8.550e-010	-9.109	-9.06
0.041	Fe_di003	2.999e-011	3.293e-011	-10.523	-10.48
0.041 Ca	1.476e-001	4 000 004		0.000	
-0.568	(a+2	1.293e-001	3.499e-002	-0.888	-1.45
0.041	Ca204	9.21/e-003	6 3960 003	-2.035	-1.99
-0.152	CarD3	9 729-006	1 068-005	-5 012	-2.15
0.041	CaHSO4+	2.999e-007	2.192e-007	-6.523	-6.65
-0.136	CaOH+	2.130e-009	1.557e-009	-8.672	-8.800
-0.136 Cl	2.367e-001				
-0.181	C1-	2.367e-001	1.559e-001	-0.626	-0.80
-0.136	MACL+	5.14'/e-008	3.761e-008	-7.288	-/.42
-0.545	re_unu+2	1.200e-008	2 395~ 000	-1.921	-8.465
-0.136	re_uriulz+ Mac12	2 3310 000	2.3830-009	_d.486	-8.62
0.041	Fe diCl+	2.224-009	1.625-009	-0.002	_8 78
-0.136	MnCl3-	1.504-010	1.099-010	-0.000	_9,950
-0.136	Fe tri(13	3.385-011	3.718-011	-10 470	-10 430
0.041 Fe_di	4.531e-008 Fe_di+2	2.648e-008	7.553e-009	-7.577	-8.122
-0.545					

_0 136	Fe_diH003+	1.481e-008	1.082e-008	-7.830	-7.966
_0.136	Fe_diCl+	2.224e-009	1.625e-009	-8.653	-8.789
0.041	Fe_diSO4	1.773e-009	1.947e-009	-8.751	-8.711
0.041	Fe_diCO3	2.999e-011	3.293e-011	-10.523	-10.482
0.136	Fe_diOH+	8.763e-013	6.404e-013	-12.057	-12.194
0.136	Fe_diH904+	6.474e-014	4.732e-014	-13.189	-13.325
0.041	Fe_di(HS)2	0.000e+000	0.000e+000	-278.065	-278.024
_0 136	Fe_di (HS) 3-	0.000e+000	0.000e+000	-415.277	-415.413
Fe_tri	1.610e-004	1 530-004	1 118-004	_3 815	_3 952
-0.136	Fe triOH+2	4 414-006	1 259-006	-5 355	-5 900
-0.545	Fe tri (OH) 3	3 516-006	3 861-006	-5 454	-5 413
0.041	Fe trig04+	1 582-008	1 156-008	-7 801	_7 937
-0.136	Fe tri+3	1 223-008	7 273-010	-7 913	-9 138
-1.226	Fe triCl+2	1.200e-008	3.424e-009	-7.921	-8.465
-0.545	Fe tri2(0H)2+4	6 442e-009	4 267-011	-8 191	-10 370
-2.179	Fe triCl2+	3.263e-009	2.385e-009	-8.486	-8.623
-0.136	Fe tri3(0H)4+5	2.530e-009	9.966e-013	-8.597	-12.001
-3.405	Fe tri (OH) 4-	1.292e-009	9.442e-010	-8,889	-9.025
-0.136	Fe tri (904)2-	5.018e-010	3.667e-010	-9.299	-9.436
-0.136	Fe triCl3	3.385e-011	3.718e-011	-10.470	-10.430
0.041	Fe triHSO4+2	4.012e-013	1.145e-013	-12.397	-12.941
-0.545 H(0)	0.000e+000	0.000e+000	0.000e+000	-44.396	-44.355
0.041 K					
-0.181	K+	5.222e-005	3.440e-005	-4.282	-4.463
-0.136	K904-	4.794e-007	3.504e-007	-6.319	-6.455
0.041	KOH	2.912e-014	3.198e-014	-13.536	-13.495
Mg	9.719e-004 Mg+2	8.365e-004	2.512e-004	-3.078	-3.600
-0.522	Mg904	7.774e-005	8.537e-005	-4.109	-4.069
0.041	MgHCO3+	5.761e-005	4.210e-005	-4.239	-4.376
-0.136	MgCO3	3.967e-008	4.356e-008	-7.402	-7.361
0.041	MgCH+	3.346e-010	2.445e-010	-9.476	-9.612
-0.136 Mn(2)	3.951e-007	0.000.007	5 000 000	6 650	5.000
-0.576	Mn+2	2.230e-007	5.922e-008	-6.652	-7.228
-0.136	MnHLUS+	1.0350-007	7.562e-008	-6.985	-/.121
-0.136	MnC1+	5.14/e-008	3.761e-008	-/.288	-7.425
0.041	MISO4	2.331- 000	1.52/e-008	-/.85/	-/.810
0.041	MIC12	2.331e-009	2.500e-009	-8.032	-8.392
0.041	MILLOS	1 504- 010	8.550e-010	-9.109	-9.068
-0.136	MILLS-	E 5050 012	1.0990-010	10.052	-9.959
-0.136	4 EEEo 017	5.5656-015	4.0028-015	-22.235	-12.309
-1.226	4.555e-017 Mn+3	4.555e-017	2.710e-018	-16.341	-17.567
. 14C	4.1830-004 Na+	4.132e-004	2.951e-004	-3.384	-3.530
-0.146	NaSO4-	2.934e-006	2.144e-006	-5.533	-5.669
-0.130	NaHCO3	2.165e-006	2.377e-006	-5.665	-5.624
0.126	NaCO3-	1.366e-009	9.986e-010	-8.864	-9.001
0.110	NaCH	4.760e-013	5.227e-013	-12.322	-12.282
O(0)	3.828e-004 02	1.914e-004	2.102e-004	-3.718	-3.677
S(-2)	0.000e+000	0 000~+000	0 000~+000	_137 057	_137 017
0.041	نك. HC_		0.000~000	חכר חבר. חכר חבר_	-130 /02
-0.187	-u- -u-	0.000-:000	0.000-:000	ענג. בנב- 146 יידי	146 012
-0.635	Fe di /ue\?		0.000~000	-140.211	_278 004
0.041	Fe di (HC) 3			_/15_277	_/15 /13
-0.136	1 579 <u>–</u> 000	5.000er000	5.000er000	<i>۱۱۵، ب</i> ید	CT6.CTE
0.041	Ca904	9.217e-003	1.012e-002	-2.035	-1.995
-0.651	904-2	6.491e-003	1.450e-003	-2.188	-2.839
0.041	MgSO4	7.774e-005	8.537e-005	-4.109	-4.069
-0.136	NaSO4-	2.934e-006	2.144e-006	-5.533	-5.669

0 100	H904-	7.130e-007	5.211e-007	-6.147	-6.283
-0.136	K904-	4.794e-007	3.504e-007	-6.319	-6.455
-0.136	CaH904+	2.999e-007	2.192e-007	-6.523	-6.659
-0.136	Fe_triSO4+	1.582e-008	1.156e-008	-7.801	-7.937
-0.136	Mn904	1.390e-008	1.527e-008	-7.857	-7.816
0.041	Fe <u>di</u> 904	1.773e-009	1.947e-009	-8.751	-8.711
0.041	Fe_tri(SO4)2-	5.018e-010	3.667e-010	-9.299	-9.436
-0.136	Fe_triH904+2	4.012e-013	1.145e-013	-12.397	-12.941
-0.545	Fe <u>diH</u> 904+	6.474e-014	4.732e-014	-13.189	-13.325
-0.136					
		-saturation i	nalces		

Phase	SI	log IAP	log KT	
Arhydrite Aragonite Calcite (C2(g) Dolamite (Gpsum H20(g) H20(g) Halite Hausnarnite Margenite (C2(g) Pyroduroite Pyrolusite Rododrosite Sulfur	$\begin{array}{c} 0.07\\ 0.14\\ 0.28\\ -138.48\\ 0.55\\ -1.45\\ 0.28\\ -41.21\\ -1.51\\ -1.592\\ -8.93\\ -1.11\\ -0.79\\ -11.57\\ 3.45\\ -2.84\\ -101.59\end{array}$	-4.29 -8.20 -8.20 -141.34 -0.92 -18.54 -4.30 -44.36 -0.00 -137.92 -4.34 52.10 24.23 -3.68 3.63 44.83 -13.97 -96.71	$\begin{array}{c} -4.36\\ -8.34\\ -8.48\\ -2.86\\ -1.47.09\\ -4.58\\ -3.15\\ 1.51\\ -1.00\\ 1.58\\ 61.03\\ 25.34\\ -2.89\\ 15.20\\ 41.38\\ -11.13\\ 4.88\end{array}$	CaSD4 CaCD3 CaCD3 C4H4 CC2 CaVbg(CC3)2 CaSD4:2H20 H2 H2O H2S Mn3C4 Mn3C4 Mn2CH Mn2CH Mn2CH Mn2CH Mn2C Mn2C3 S

Reaction step	98.
WARNING: Elen	nent Fe_di has negative moles in solution, -2.872895e-008. Erroneous mole balance occurs as moles are added to produce
zero moles.	Usually caused by KINETICS, REACTION, or diffuse layer
calculation. simulation or WARNING: Elem	May be due to large time steps in early part of KINEIICS r negative concentrations in the diffuse layer. nent Re_di has negative moles in solution, -1.971399e-009.
zero moles.	Erroneous mole balance occurs as moles are added to produce
calculation.	Marche du te leure time terre in enderent of Mature
simulation or WARNING: Elen	ray be due to large the steps in early part of Anterics regative concentrations in the diffuse layer. earlt Fe_di has negative moles in solution, -3.030945e-009. Erroneous mole balance occurs as moles are added to produce
zero moles.	Usually caused by KINETICS, REACTION, or diffuse layer
simulation or	May be due to large time steps in early part of KINETICS regetive concentrations in the diffuse layer, metric and the persenting relation collision 2.416660,000
WARDING: FIG	Erroneous mole balance occurs as moles are added to produce
zero notes.	Usually caused by KINETICS, REACTION, or diffuse layer
simulation or	May be due to large time steps in early part of KINETICS regative concentrations in the diffuse layer.
WARNING: EIG	Tent Fe_on has negative moles in solution, -1.4/86.22e-009. Erroneous nole balance occurs as noles are added to produce
zero moies.	Usually caused by KINETICS, REACTION, or diffuse layer
simulation or WARNING: Elem	May be due to large time steps in early part of KINETICS regative concentrations in the diffuse layer. rent Fe_di has negative noles in solution, -7.499156e-010. Erromeous mole balance occurs as moles are added to produce
zero moles.	- Usually caused by KINETICS, REACTION, or diffuse layer
calculation.	May be due to large time steps in early part of KINETICS
simulation or WARNING: Elen	: négative concentrations in the diffuse layer. nent Fe_di has negative moles in solution, -3.589512e-011. Erroneous mole balance occurs as moles are added to produce
zero moles.	Usually caused by KINETICS, REACTION, or diffuse layer
calculation.	May be due to large time steps in early part of KINETICS
Using solution	n 1. nase assemblage 1.
Using kinetic	s 1. Kinetics defined in simulation 2.
Kinetics 1.	Kinetics defined in simulation 2.
	Time step: 172800 seconds (Incremented time: 345600 seconds)
Coefficient	Rate name Delta Moles Total Moles Reactant
-1	Fe_di_ax -4.530e-008 9.998e-001 Fe_di
1	Fe_tri
	Phase assemblage
-	Malon in another
Delta	Phase SI log IAP log KT Initial Final
	C2(g) -0.78 -3.68 -2.89 1.000e+001 1.000e+001-

1.132e-008

		Solution comp	osition			
	Elements	Molality	Moles			
	C Ca Cl Fe_di Fe_tri K Mg Mg Na S	1.389e-001 1.476e-001 2.367e-001 1.298e-011 1.610e-004 5.270e-005 9.719e-004 3.951e-007 4.183e-004 1.579e-002	1.389e-001 1.476e-001 2.367e-001 1.298e-011 1.610e-004 5.270e-005 9.719e-004 3.951e-007 4.183e-004 1.579e-002			
	D	escription of	solution			
		pH pe	= 5.432 = 15.170	Charge Adiust	e balance ed to redox	
pe = 15.17.0 Adjusted to redox equilibrium Activity of water = 0.991 Ionic strength = 4.066e-001 Mess of water (kg) = 1.000e+000 Total alkalinity (eg/kg) = 2.983e-002 Total 002 (m0/kg) = 1.389e-001 Tapperature (deg C) = 25.000 Electrical halance (eg) = -1.264e-009 Percent error, 100*(Cat-[An])/(Cat+[An]) = -0.00 Iterations = 236 Total H = 1.110421e+002 Total 0 = 5.587731e+0001						
	D	istribution o	of species			
				Log	Log	
Log	Species	Molality	Activity	Molality	Activity	
Ganma	TT.	4 701- 000	2 607- 000	E 200	- E 400	
-0.113	11+ (1H-	4./910-006	3.69/e-006	-5.320 _8.384	-5.4 <i>3</i> 2 _8 571	
-0.187		5.551e+001	9.911e-001	1.744	-0.004	
0.000 ⊂(-4)	0.000e+000	0.000 000	0.000 005	141.007	141 242	
0.041	CH4 1 389-001	0.000e+000	0.000e+000	-141.384	-141.343	
2(⊈) ).041	02	1.094e-001	1.201e-001	-0.961	-0.920	
-0.152	HCO3-	2.035e-002	1.433e-002	-1.691	-1.844	
-0.152	CaHCO3+	9.085e-003	6.396e-003	-2.042	-2.194	
-0.136	MgHCO3+	5.761e-005	4.210e-005	-4.239	-4.376	
0.041	NaHOO3	9.729e-006	2.377e-006	-5.665	-4.971	
0.041	003-2	7.400e-007	1.818e-007	-6.131	-6.741	
-0.610	MnHCO3+	1.035e-007	7.562e-008	-6.985	-7.121	
-0.136	MgC03	3.967e-008	4.356e-008	-7.402	-7.361	
0.126	NaCO3-	1.366e-009	9.986e-010	-8.864	-9.001	
0.130	MinCO3	7.786e-010	8.550e-010	-9.109	-9.068	
-0.136	Fe_diHCO3+	4.243e-012	3.101e-012	-11.372	-11.509	
0.041	Fe_diCO3	8.593e-015	9.436e-015	-14.066	-14.025	
Ъ 	1.476e-001 Ca+2	1.293e-001	3.499e-002	-0.888	-1.456	
-0.568	Ca904	9.217e-003	1.012e-002	-2.035	-1.995	
0.152	CaHCO3+	9.085e-003	6.396e-003	-2.042	-2.194	
-0.152 ) 041	CaCO3	9.729e-006	1.068e-005	-5.012	-4.971	
-0.136	CaHSO4+	2.999e-007	2.192e-007	-6.523	-6.659	
-0.136	CaOH+	2.130e-009	1.557e-009	-8.672	-8.808	
1	2.367e-001 Cl-	2.367e-001	1.559e-001	-0.626	-0.807	
-0.181	MnCl+	5.147e-008	3.761e-008	-7.288	-7.425	
-0.130	Fe_triCl+2	1.201e-008	3.425e-009	-7.921	-8.465	
-0.136	Fe_triCl2+	3.264e-009	2.385e-009	-8.486	-8.622	
0.041	MnC12	2.331e-009	2.560e-009	-8.632	-8.592	
-0.136	MnCl3-	1.504e-010	1.099e-010	-9.823	-9.959	
0.041	Fe_triCl3	3.386e-011	3.719e-011	-10.470	-10.430	
-0.136	Fe_diCl+	6.373e-013	4.658e-013	-12.196	-12.332	
re <u>di</u>	1.298e-011 Fe_di+2	7.587e-012	2.164e-012	-11.120	-11.665	
-0.345	Fe_diH003+	4.243e-012	3.101e-012	-11.372	-11.509	
-0.136	Fe_diCl+	6.373e-013	4.658e-013	-12.196	-12.332	
0.041	Fe_diSO4	5.081e-013	5.580e-013	-12.294	-12.253	

0.041	Fe_diC03	8.593e-015	9.436e-015	-14.066	-14.025
0.041	Fe_diOH+	2.511e-016	1.835e-016	-15.600	-15.736
-0.136	Fe_diH904+	1.855e-017	1.356e-017	-16.732	-16.868
-0.136	Fe_di(HS)2	0.000e+000	0.000e+000	-281.608	-281.567
0.041	Fe_di (HS) 3-	0.000e+000	0.000e+000	-418.820	-418.956
-0.136 Fe_tri	1.610e-004	1 5300 004	1 119- 004	3 915	3 051
-0.136	Fe_triOH+2	4 415e-006	1 259-004	-5.355	-5.900
-0.545	Fe tri (OH) 3	3 517-006	3 862-006	-5 454	_5 /13
0.041	Fo trigo/+	1 5930 009	1 1570 008	7 901	7 037
-0.136	Te_crisoar	1 2220 000	7 275- 010	7 012	0 120
-1.226	Fe_tri=5	1.2230-000	7.275e-010	7.001	-9.130
-0.545	Fe_trici+2	6 4460 000	3.425e-009	-7.921 0.101	-8.400
-2.179	Fe_triz(0ri)2+4	0.4400-009	4.209e-011	-0.191	-10.370
-0.136	Fe_triciz+	3.2040-009	2.3850-009	-8.480	-8.022
-3.405	Fe_tr13(UH)4+5	2.532e-009	9.9/4e-013	-8.597	-12.001
-0.136	Fe_tri (OH) 4-	1.292e-009	9.444e-010	-8.889	-9.025
-0.136	Fe_tri (904) 2-	5.020e-010	3.6680-010	-9.299	-9.436
0.041	Fe_tricl3	3.3860-011	3./190-011	-10.470	-10.430
-0.545	Fe_triH904+2	4.013e-013	1.145e-013	-12.397	-12.941
H(0)	H2	0.000e+000	0.000e+000	-44.396	-44.355
K	5.270e-005	5.222e-005	3.440e-005	-4.282	-4.463
-0.181	KdO1-	4 794-007	3 50/0-007	_6 319	_6 /155
-0.136	KOH	2 912-014	3 198-014	-13 536	-13 495
0.041 Mar	9.719e-004	2.9120 014	5.1500 014	19:550	10.400
-0.522	Mg+2	8.365e-004	2.512e-004	-3.078	-3.600
0.041	Mg904	7.774e-005	8.537e-005	-4.109	-4.069
-0.136	MgHCO3+	5.761e-005	4.210e-005	-4.239	-4.376
0.041	MgCO3	3.967e-008	4.356e-008	-7.402	-7.361
-0.136	MgCH+	3.346e-010	2.445e-010	-9.476	-9.612
Mn(2)	3.951e-007 Mp+2	2 230e-007	5 922-008	-6 652	-7 228
-0.576	MoHOO3+	1 035-007	7 562-008	_6.985	_7 121
-0.136	Mecl+	5 1470 009	3 7610 009	7 200	7 /25
-0.136	Maccol	1 200- 009	1 527- 000	7 057	7 016
0.041	M1304	2.331- 000	2.5270-000	-7.007	-7.010
0.041	MIC12	2.551e-009	2.3008-009	-0.032	-0.052
0.041	MhLO3	/./866-010	8.5508-010	-9.109	-9.068
-0.136	MnCL3-	1.504e-010	1.099e-010	-9.823	-9.959
-0.136 Mp(3)	MnOH+ 4 555e-017	5.585e-013	4.082e-013	-12.253	-12.389
-1.226	Mn+3	4.555e-017	2.710e-018	-16.341	-17.567
Na	4.183e-004 Na+	4.132e-004	2.951e-004	-3.384	-3.530
-0.146	Na904-	2.934e-006	2.144e-006	-5.533	-5.669
-0.136	Nahoos	2 165-006	2 377-006	-5 665	-5 624
0.041	NaCO3-	1 366-009	9 986-010	-8 864	_9 001
-0.136	NaCH	4 760e-013	5 227e-013	-12 322	-12 282
0.041 O(0)	3.828e-004				
0.041	02	1.914e-004	2.102e-004	-3.718	-3.677
S(-2)	0.000e+000 H2S	0.000e+000	0.000e+000	-137.957	-137.917
0.041	HS-	0.000e+000	0.000e+000	-139.239	-139.426
-0.187	S-2	0.000e+000	0.000e+000	-146.277	-146.912
-0.635	Fe_di(HS)2	0.000e+000	0.000e+000	-281.608	-281.567
0.041	Fe_di(HS)3-	0.000e+000	0.000e+000	-418.820	-418.956
=0.136 S(6)	1.579e-002	9 2170 003	1 0120 002	2 035	1 005
0.041	901_2	6 /191~ 003	1 450- 002	-2.033	-2 020
-0.651	104-2 Mag2/	7 77/~ 005	2.5370 005		_2.039
0.041	Na90/-	2 92/10 005	2 1000	-2 233	-4.009
-0.136	H904-	7 130-007	5 211-007	_6 1/7	-6.262
-0.136	K904-	4 79/2 007	3 50/10 007	-0.14/ _6 210	-0.203
-0.136	CaH904+	2 999-007	2 192-007	-6 523	-6 650
-0.136	and the second s	2		0.20	0.009

0 126	Fe <u>tri</u> SO4+	1.583e-008	1.157e-008	-7.801	-7.937
-0.130	MnSO4	1.390e-008	1.527e-008	-7.857	-7.816
0.126	Fe_tri(SO4)2-	5.020e-010	3.668e-010	-9.299	-9.436
-0.130	Fe_diSO4	5.081e-013	5.580e-013	-12.294	-12.253
0.041	Fe_triH904+2	4.013e-013	1.145e-013	-12.397	-12.941
_0.136	Fe_diH904+	1.855e-017	1.356e-017	-16.732	-16.868
		Saturation i	ndices		

Phase	SI log IAP	log KT	
Anhydrite Aragonite Calcite CAlcite CA4(g) Dolonite Gypsum H2(g) H20(g)	0.07 -4.29 0.14 -8.20 0.28 -8.20 -138.48 -141.34 0.55 -0.92 -1.45 -18.54 0.28 -4.30 -41.21 -44.36 -1.51 -0.00	-4.36 -8.34 -8.48 -2.86 -1.47 -17.09 -4.58 -3.15 1.51	CaSO4 CaCO3 CaCO3 CH4 CO2 CaMg(CC3)2 CaSO4:2H2O H2 H2O
H2S(g) Halite Hausmannite Manganite Q2(g) Pyroducite Pyrolusite Rhodochrosite Sulfar	-136.92 -137.92 -5.92 -4.34 -8.93 52.10 -1.11 24.23 -0.78 -3.68 -11.57 3.63 3.45 44.83 -2.84 -13.97 101 59 96 71	-1.00 1.58 61.03 25.34 -2.89 15.20 41.38 -11.13	H2S NaCl Mn3O4 MnOOH O2 Mn(OH)2 MnO2 MnO2 S

	Rhodochrosite Sulfur	-2.84 -101.59	-13.97 -96.71	-11.13 4.88	MhCO3 S
Reaction step	o 9.				
WARNING: Elen	rent Fe_di has ne	gative m	les in :	solution	, -8.232164e-012.
zero moles.	Erroneous mole l	balance c	ocurs a:	s moles	are added to produce
calculation.	Usually caused I	by KINEFI	CS, REA	CTION, O	r diffuse layer
simulation or WARNING: Elem	May be due to la regative concent ment Fe_di has ne Fromeous mole l	arge time trations gative mo balance o	in the oles in a	in early diffuse solution	part of KINETICS layer. , -5.648819e-013. are added to produce
zero moles.	Usually caused	by KINETT	OS REM		r diffuse laver
calculation.	Marko dia ta li	oy Idiwili			r arriver af VINUTOC
simulation or WARNING: Elem	negative concen nent Fe_di has ne Fromeous mole l	trations gative m balance c	in the o les in a	diffuse solution	layer. 18.685081e-013. are added to produce
zero moles.	Uranily cauced i				r diffuso larger
calculation.	May be due to 1	avro tim		in onclu	r arriade layer
simulation or WARNING: Elem	negative concen nent Fe_di has ne Fromeous mole l	trations gative mo balance c	in the o les in a	diffuse solution	layer. 1, -6.920311e-013.
zero moles.	Usually caused l	by KINEPI	CS. REA	TTON. O	r diffuse laver
calculation.	Marcho duo to li	avro timo		in oarlu	nert of KINKUICS
simulation or WARNING: Elem	r negative concen nent Fe_di has ne Fromeous mole l	trations gative m balance c	in the o les in a	diffuse solution	layer. 1, -4.236973e-013.
zero moles.	Denally caused l	by KINETT	NAR 20		r diffuse laver
calculation.	May be due to 1	avro tim		in onclu	r arriade layer
simulation or WARNING: Elem	negative concen nent Fe_di has ne Fromeous mole l	trations gative m balance c	in the o les in a	diffuse solution	layer. 1, -2.148874e-013.
zero moles.	Denally caused l	by KINETT	NAR 20		r diffuse laver
calculation.	May be due to 1	amo timo	etane :	in carly	rant of KINFUICS
simulation or WARNING: Elem	regative concen rent Fe_di has ne Erronecus mole l	trations gative mo balance c	in the o les in a cours a	diffuse solution s moles	layer. 1, -1.028570e-014. are added to produce
zero moles.	Usually caused I	by KINEFI	CS, REA	CTION, o	r diffuse layer
calculation.	May be due to la	- arge time	steps :	in early	part of KINEFICS
simulation or Using solution Using pure ph	r negative concen m 1. nase assemblage 1	trations	in the (	diffuse	layer.
Using kinetic	351. K	inetics d	etined i	in simuli	ation 2.
Kinetics 1.	Kinetics define	d in simu	lation 2	2.	
	Time step: 1728	00 second	ls (Inci	remented	time: 518400 seconds)
Coefficient	Rate name	Delta Mc	les Tota	al Moles	Reactant
-1	Fe <u>di</u> ax	-1.298e-	011 9.9	998e-001	Fe <u>di</u>
1					Fe_tri
		Phase a	sembla	ne	
				5-	
Delta	Phase	SI 1	og IAP	log KT	Moles in assemblage Initial Final
3.196e-012	O2 (g)	-0.78	-3.68	-2.89	1.000e+001 1.000e+001-
		Solution	canposi	tion	
	Florents	14-1-1	itar	Mole-	
	malaits	roudi	тсу.	rotes	

	C Ca Cl Fe_cti Fe_tri K Mg Mn Na S	1.389e-001 1.476e-001 2.367e-001 3.720e-015 1.610e-004 5.270e-005 9.719e-004 3.951e-007 4.183e-004 1.579e-002	1.389e-001 1.476e-001 2.367e-001 3.720e-015 1.610e-004 5.270e-005 9.719e-004 3.951e-007 4.183e-004 1.579e-002		
	D	escription of	solution		
equilibrium	Activ Io Mass o Total alkali Total (	pH pe nic strength f water (kg) nity (eq/kg) 002 (mol/kg)	= 5.432 = 15.170 = 0.991 = 4.066e-( = 1.000e+( = 2.983e-( = 1.389e-(	Charge Adjust 001 000 002 001	e bal <i>a</i> nce ied to redox
Percent erro	Tempera Electrical l or, 100*(Cat- An	ture (deg C) balance (eg) )/(Cat+ An ) Iterations Total H Total O	$= 25.000 \\= -1.265e-( \\= -0.00 \\= 233 \\= 1.110421e \\= 5.587731e \\$	009 2+002 2+001	
	<u></u> u		DI Species		
Log				Log	Log
Ganma	Species	Molality	Activity	Molality	Activity
	H+	4.791e-006	3.697e-006	-5.320	-5.432
-0.113	OH-	4.133e-009	2.684e-009	-8.384	-8.571
-0.18/	H2O	5.551e+001	9.911e-001	1.744	-0.004
C(-4)	0.000e+000 CH4	0.000e+000	0.000e+000	-141.384	-141.343
C(4)	1.389e-001 CC2	1.094e-001	1.201e-001	-0.961	-0.920
0.041	H003-	2.035e-002	1.433e-002	-1.691	-1.844
-0.152	CaHCO3+	9.085e-003	6.396e-003	-2.042	-2.194
-0.152	MgHCO3+	5.761e-005	4.210e-005	-4.239	-4.376
-0.136	CaCO3	9.729e-006	1.068e-005	-5.012	-4.971
0.041	NaHCO3	2.165e-006	2.377e-006	-5.665	-5.624
0.041	003-2	7.400e-007	1.818e-007	-6.131	-6.741
-0.610	MnHCO3+	1.035e-007	7.562e-008	-6.985	-7.121
0.041	MgCO3	3.967e-008	4.356e-008	-7.402	-7.361
-0.136	NaCO3-	1.366e-009	9.986e-010	-8.864	-9.001
0.041	MinCO3	7.786e-010	8.550e-010	-9.109	-9.068
-0.136	Fe_diH003+	1.216e-015	8.885e-016	-14.915	-15.051
0.041	Fe_diCO3	2.462e-018	2.704e-018	-17.609	-17.568
Ca	1.476e-001 Ca+2	1.293e-001	3.499e-002	-0.888	-1.456
-0.568	Ca304	9.217e-003	1.012e-002	-2.035	-1.995
0.041	CaHCO3+	9.085e-003	6.396e-003	-2.042	-2.194
-0.152	CaCO3	9.729e-006	1.068e-005	-5.012	-4.971
0.041	CaHSO4+	2.999e-007	2.192e-007	-6.523	-6.659
-0.136	CaCH+	2.130e-009	1.557e-009	-8.672	-8.808
ci	2.367e-001 Cl-	2.367e-001	1.559e-001	-0.626	-0.807
-0.181	MnCl+	5.147e-008	3.761e-008	-7.288	-7.425
-0.136	Fe_triCl+2	1.201e-008	3.425e-009	-7.921	-8.465
-0.545	Fe_triCl2+	3.264e-009	2.385e-009	-8.486	-8.622
-0.136	MnCl2	2.331e-009	2.560e-009	-8.632	-8.592
0.041	MnCl3-	1.504e-010	1.099e-010	-9.823	-9.959
-0.136	Fe_triCl3	3.386e-011	3.719e-011	-10.470	-10.430
J.U41	Fe_diCl+	1.826e-016	1.335e-016	-15.738	-15.875
Fe_di	3.720e-015 Fe_di+2	2.174e-015	6.202e-016	-14.663	-15.207
-0.545	Fe_diH003+	1.216e-015	8.885e-016	-14.915	-15.051
-0.136	Fe_diCl+	1.826e-016	1.335e-016	-15.738	-15.875
-0.136	Fe_diSO4	1.456e-016	1.599e-016	-15.837	-15.796
0.041	Fe_di003	2.462e-018	2.704e-018	-17.609	-17.568
0.136	Fe_diOH+	7.195e-020	5.258e-020	-19.143	-19.279
-0.136	Fe_diH904+	5.316e-021	3.885e-021	-20.274	-20.411

	Fe_di(HS)2	0.000e+000	0.000e+000	-285.150	-285.110	
0.041	Fe <u>di</u> (HS)3-	0.000e+000	0.000e+000	-422.363	-422.499	
-0.136 Fe <u>t</u> ri	1.610e-004	1 5300 004	1 119- 004	3 915	3 951	
-0.136	Fe_UII (UR) 2+	1.5508-004	1 259-004	-5.815	-5.900	
-0.545	Fe tri (OH) 3	3 517-006	3 862-006	_5.454	_5 /13	
0.041	Fe trig0/+	1 583-008	1 157-008	_7 801	_7 937	
-0.136	Fe tri+3	1 223-008	7 275-010	_7 913	_9 138	
-1.226	Fe triCl+2	1 201-008	3 425-009	-7 921	-8 465	
-0.545	Fe tri2(0H)2+4	6 446-009	4 269-011	-8 191	-10 370	
-2.179	Fe triCl2+	3 264-009	2 385-009	-8 486	-8 622	
-0.136	Fe tri3(0H)4+5	2.532e-009	9.974e-013	-8,597	-12.001	
-3.405	Fe tri (OH) 4-	1.292e-009	9.444e-010	-8,889	-9.025	
-0.136	Fe tri (SO4)2-	5.020e-010	3.668e-010	-9.299	-9.436	
-0.136	Fe triCl3	3.386e-011	3.719e-011	-10.470	-10.430	
0.041	Fe triHSO4+2	4.013e-013	1.145e-013	-12.397	-12,941	
-0.545 H(0)	0.000e+000					
0.041	H2	0.000e+000	0.000e+000	-44.396	-44.355	
K	5.270e-005 K+	5.222e-005	3.440e-005	-4.282	-4.463	
-0.181	K904-	4.794e-007	3.504e-007	-6.319	-6.455	
-0.136	KOH	2.912e-014	3.198e-014	-13.536	-13.495	
0.041 Mg	9.719e-004					
-0.522	Mg+2	8.365e-004	2.512e-004	-3.078	-3.600	
0.041	Mg904	7.774e-005	8.537e-005	-4.109	-4.069	
-0.136	MgHCO3+	5.761e-005	4.210e-005	-4.239	-4.376	
0.041	MgCO3	3.967e-008	4.356e-008	-7.402	-7.361	
-0.136	MgCH+	3.346e-010	2.445e-010	-9.476	-9.612	
Mn(2)	3.951e-007 Mn+2	2.230e-007	5.922e-008	-6.652	-7.228	
-0.5/6	MnHCO3+	1.035e-007	7.562e-008	-6.985	-7.121	
0.136	MnCl+	5.147e-008	3.761e-008	-7.288	-7.425	
0.011	MnSO4	1.390e-008	1.527e-008	-7.857	-7.816	
0.041	MnCl2	2.331e-009	2.560e-009	-8.632	-8.592	
0.041	MnCO3	7.786e-010	8.550e-010	-9.109	-9.068	
-0.136	MnCl3-	1.504e-010	1.099e-010	-9.823	-9.959	
-0.136	MnOH+	5.585e-013	4.082e-013	-12.253	-12.389	
Mn(3)	4.555e-017 Mn+3	4.555e-017	2.710e-018	-16.341	-17.567	
-1.226 Na	4.183e-004		0.054.004		0.500	
-0.146	Na+	4.132e-004	2.951e-004	-3.384	-3.530	
-0.136	Naso4-	2.9340-006	2.1440-000	-5.555	-5.009	
0.041	Nahuus	2.105e-000	2.37/e-006	-3.005	-5.624	
-0.136	Naccu	1.3000-009	5 2270 013	10.004	12 292	
0.041	3 828-004	4.7008-015	J.22/8-01J	-12.322	-12.202	
0.041	02	1.914e-004	2.102e-004	-3.718	-3.677	
S(-2)	0.000e+000 H2S	0.000e+000	0.000e+000	-137.957	-137.917	
0.041	HS-	0.000e+000	0.000e+000	-139.239	-139.426	
-0.187	S-2	0.000e+000	0.000e+000	-146.277	-146.912	
-0.635	Fe_di(HS)2	0.000e+000	0.000e+000	-285.150	-285.110	
0.041	Fe_di (HS) 3-	0.000e+000	0.000e+000	-422.363	-422.499	
-0.136 S(6)	1.579e-002	0.045 000	4 040 000	0.005	4 005	
0.041	CO1 2	9.21/e-003	1.012e-002	-2.035	-1.995	
-0.651	504-2 M6004	0.491e-003	1.450e-003	-2.188	-2.839	
0.041	ng504 N5004	1.1/4e-005	0.03/e-005	-4.109	-4.069	
-0.136	1100/4-	2.9340-000	2.1440-000	-0.000	-3.669	
-0.136	1204-	1.130e-007	3 504~ 007	-0.14/	-0.203	
-0.136	CaHGO(+	2 999~ 007	2 192~ 007	-6 577	-0.400	
-0.136	Fe trigN+	1 583a 00P	1 157~ 000	Q01	-0.009	
-0.136	Mh904	1 390-000	1 527~000	_7 857	-7 816	
0.041	Fe tri (904)?-	5.020-010	3.668-010	_9 299	-9.436	
-0.136	,,					

	Fe triH901+2	4 013-013	1 1/5-013	_12 397	_12 9/1
-0.545	Fe dis04	1.456e-016	1.599e-016	-15.837	-15.796
0.041	Fe_diH904+	5.316e-021	3.885e-021	-20.274	-20.411
-0.136					
		-Saturation ir	ndices		
	Phase	SI log IZ	P log KT		
	Arhydrite Aragonite Calcite C44(g) C02(g) Dolomite Cypsum H2(g) H25(g) Halite Hausmanite Marganite O2(g) Pyroduroite Pyrolusite Rodochrosite Sulfur	0.07 4.2 0.14 -8.2 0.28 -8.2 -1.38.48 -141.3 0.55 -0.2 -1.45 -1.8.5 0.28 -4.3 -1.51 -0.0 -136.92 -137.9 -4.21 -44.3 -5.92 -4.3 -8.93 52.1 -1.11 24.2 -0.78 -3.6 -11.57 3.6 -11.57 3.6 -11.57 -3.6 -101.59 -96.3	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	CaSO4 CaCO3 CaCO3 CACO3 CACO3 CACG CASO4:2H2O H2 H2O H2S H2O H2S H2O H2S H2O H2O H2O H2O H2O H2O H2O H2O H2O H2O	
Reaction ste	p 10.			-	
WARNING: Ele	ment Fe_di has ne	gative moles :	in solution,	-2.3589176	-015.
zero moles.	Erroneous mole	balance occurs	s as moles a	re added to	produce
calculation.	Usually caused	by KINEFICS, F	REACTION, or	diffuse la	yer
simulation of WARNING: Elem	May be due to 1 r negative concer ment Fe_di has ne Formeous mole	arge time ster trations in th gative moles : balance corum	ne diffuse l in solution,	part of Kilv ayer. -1.618662e	EFICS ←016.
zero noles.	Usually caused	by KINETICS. F	FACTION. Or	diffuse la	ver
calculation.	May be due to 1	arge time ster	s in early	part of KIN	EFICS
simulation o WARNING: Ele	r negative concer ment Fe_di has ne Erroneous mole	trations in t gative moles : balance occurs	ne diffuse l in solution, s as moles a	ayer. -2.488700e re added to	÷-016. o produce
zero moles.	Usually caused	by KINEFICS, F	EACTION, or	diffuse la	yer
calculation. simulation or WARNING: Eler	May be due to l r negative concer ment Fe_di has ne Enronecus mole	arge time ster trations in th gative moles i balance occurs	ps in early ne diffuse l in solution, s as moles a	part of KIN ayer. -1.983007e re added to	EFICS +-016.
zero moles.	Usually caused	by KINEFICS, F	REACTION, or	diffuse la	ver
calculation. simulation of WARNING: Elec	May be due to l r negative concer ment Fe_di has ne	arge time ster trations in the gative moles :	ps in early ne diffuse l in solution,	part of KIN ayer. -1.214100e	-016 <u>.</u>
zero moles.	Erroneous mole	balance occurs	sas molesa Tenormoni or	re accec to	) produce
calculation.	May be due to 1	avone time stor	re in carly:	nart of KTN	iver.
simulation o WARNING: Eler	r negative concer ment Fe_di has na Erroneous mole	trations in the gative moles : balance occurs	ne diffuse l in solution, s as moles a	ayer. -6.157574a re added to	÷017. ⇒ produce
zero moles.	Usually caused	by KINEFICS, F	REACTION, or	diffuse la	yer
calculation. simulation or WARNING: Eler	May be due to l r negative concer ment Fe_di has ne	arge time ster trations in th gative moles :	ps in early ne diffuse l in solution,	part of KIN ayer. -2.9473576	ETICS
zero moles.	Erroneous mole	balance occurs	sas moles a	re added to	) produce
calculation.	May be due to 1	aven timo stor	en in carly:	carriese is	iver.
simulation o Using solutio Using pure pl	n negative concer on 1. hase assemblage 1	trations in th	ne diffuse l	ayer.	5103
Kinetics 1	Kinetics dofi-	d in similation	a in simula m 2	uun 2.	
matuto 1.	Time step: 1728	00 seconds (1	incremented	time: 69120	() seconds)
a	Rate name	Delta Moles 1	Iotal Moles	Reactant	
Operficient	Fe di av	-3.886-015	9 998-001	Fe di	
-1	re <u>ur</u> ax	-3.0006-013	9.9908-001	Fe tri	
1					
		Phase assemi	olage		
Delta	Phase	SI log IA	P log KT	bles in ass Initial	emblage Final
1.048e-013	02 (g)	-0.78 -3.6	58 -2.89 1	.000e+001 1	.000e+001
		Solution compo	osition		
	Elements	Molality	Moles		
	C C	1.389e-001	1.389e-001		
	Ca Cl	1.476e-001 2.367e-001	1.476e-001 2.367e-001		
	re <u>cu</u> Fe_tri K	1.000e-018 1.610e-004 5.270e-005	1.000e-018 1.610e-004 5.270e-005		

	Mg Mn Na S	9.719e-004 3.951e-007 4.183e-004 1.579e-002	9.719e-004 3.951e-007 4.183e-004 1.579e-002		
	De	scription of	solution		
		pH pe	= 5.432 = 15.170	Charge Adjust	e balance ied to redox
equilibrium	Activi	ty of water	= 0.991		
Percent erro	Iar Mass of Total alkalir Total C Tenperat Electrical h pr, 100*(Cat- An )	ic strength water (kg) ity (eg/kg) 02 (mol/kg) ure (deg C) alance (eg) /(Cat+[An]) Iterations Total H	$\begin{array}{r} = 4.066e+0\\ = 1.000e+0\\ = 2.983e+0\\ = 1.389e+0\\ = 25.000\\ = -1.265e+0\\ = -0.00\\ = 233\\ = 1.110421e\\ = 5.077234\end{array}$	01 000 002 001 009 =+002	
	Di	ctribution o	= 5.367/316	HUUI	
	DI	SUPIDULION C	i species		
Ior				Log	Log
Camma	Species	Molality	Activity	Molality	Activity
Claimer	H+	4.791e-006	3.697e-006	-5.320	-5.432
-0.113	0H-	4.133e-009	2.684e-009	-8.384	-8.571
-0.187	H2O	5.551e+001	9.911e-001	1.744	-0.004
0.000 C(-4)	0.000e+000				
0.041	CH4	0.000e+000	0.000e+000	-141.384	-141.343
C(4)	1.389e-001	1.094e-001	1.201e-001	-0.961	-0.920
0.041	HT03-	2 035e-002	1 433-002	-1 691	-1 844
-0.152	CaHOO3+	9 085e-003	6 3960-003	-2 042	-2 194
-0.152	MaHCO3+	5.761e-005	4.210e-005	-4.239	-4.376
-0.136	വന്ദ്	9 729-006	1 068-005	-5 012	_1 971
0.041	NHOR	2 1650 006	2 2770 006	5.012 E 66E	4.971 E 604
0.041	Nancos	2.1000-000	2.3770-000	-5.005	-5.024
-0.610	03-2	7.400e-007	1.8186-007	-6.131	-6./41
-0.136	MnHCO3+	1.035e-007	7.562e-008	-6.985	-7.121
0.041	MgCO3	3.967e-008	4.356e-008	-7.402	-7.361
-0.136	NaCO3-	1.366e-009	9.986e-010	-8.864	-9.001
0.041	MinCO3	7.786e-010	8.550e-010	-9.109	-9.068
-0.136	Fe_diHCO3+	3.484e-019	2.546e-019	-18.458	-18.594
0.041	Fe_diCO3	7.056e-022	7.748e-022	-21.151	-21.111
Ca	1.476e-001 Ca+2	1.293e-001	3.499e-002	-0.888	-1.456
-0.568	Ca904	9.217e-003	1.012e-002	-2.035	-1.995
0.041	CaHOO3+	9.085e-003	6.396e-003	-2.042	-2.194
-0.152	CaCO3	9.729e-006	1.068e-005	-5.012	-4.971
0.041	CaH904+	2 999-007	2 192-007	-6 523	-6 659
-0.136	CaOH+	2 130-009	1 557-009	_8 672	_8.808
-0.136	2 3670 001	2.1500 005	1.55/0 005	0.072	0.000
0.101	Cl-	2.367e-001	1.559e-001	-0.626	-0.807
-0.101	MnCl+	5.147e-008	3.761e-008	-7.288	-7.425
-0.136	Fe_triCl+2	1.201e-008	3.425e-009	-7.921	-8.465
-0.545	Fe_triCl2+	3.264e-009	2.385e-009	-8.486	-8.622
-0.136	MnCl2	2.331e-009	2.560e-009	-8.632	-8.592
0.041	MnCl3-	1.504e-010	1.099e-010	-9.823	-9.959
-0.136	Fe_triCl3	3.386e-011	3.719e-011	-10.470	-10.430
0.041	Fe_diCl+	5.233e-020	3.824e-020	-19.281	-19.417
-0.136 Fe_di	1.066e-018	C 000 010	1 000 010	10 000	10 750
-0.545	Fe <u>d</u> 1+2	6.230e-019	1.7//e-019	-18.206	-18.750
-0.136	re_d1HCO3+	3.484e-019	2.546e-019	-18.458	-18.594
-0.136	Fe_diCl+	5.233e-020	3.824e-020	-19.281	-19.417
0.041	Fe_diSO4	4.172e-020	4.582e-020	-19.380	-19.339
0.041	Fe_diCO3	7.056e-022	7.748e-022	-21.151	-21.111
-0.136	Fe_diOH+	2.062e-023	1.507e-023	-22.686	-22.822
-0.136	Fe_diH904+	1.523e-024	1.113e-024	-23.817	-23.953
0.041	Fe_di(HS)2	0.000e+000	0.000e+000	-288.693	-288.653
-0.136	Fe_di(HS)3-	0.000e+000	0.000e+000	-425.906	-426.042
Fe_tri	1.610e-004 Fe tri (0H)2+	1.530-004	1.118-004	_3 215	_3 951
-0.136				5.015	5.201

_0 5/15	Fe_triOH+2	4.415e-006	1.259e-006	-5.355	-5.900
0.041	Fe_tri(OH)3	3.517e-006	3.862e-006	-5.454	-5.413
0.041	Fe_tri904+	1.583e-008	1.157e-008	-7.801	-7.937
-0.136	Fe_tri+3	1.223e-008	7.275e-010	-7.913	-9.138
-1.226	Fe_triCl+2	1.201e-008	3.425e-009	-7.921	-8.465
-0.545	Fe_tri2(0H)2+4	6.446e-009	4.269e-011	-8.191	-10.370
-2.179	Fe_triCl2+	3.264e-009	2.385e-009	-8.486	-8.622
-0.136	Fe tri3(0H)4+5	2.532e-009	9.974e-013	-8.597	-12.001
-3.405	Fe tri (OH) 4-	1.292e-009	9.444e-010	-8,889	-9.025
-0.136	Fe tri (904)2-	5.020e-010	3.668e-010	-9.299	-9.436
-0.136	Fe trif13	3 386-011	3 719-011	-10 470	-10 430
0.041	Fe triH904+2	4 0130-013	1 1/50-013	_12 397	_12 9/1
-0.545	0.000-1000	4.0106-010	1.1456-015	-12.327	-12.941
0.041	H2	0.000e+000	0.000e+000	-44.396	-44.355
K K	5.270e-005	E 222- 00E	3 440- 00E	4 202	4.400
-0.181	K+	5.222e-005	3.440e-005	-4.282	-4.463
-0.136	K904-	4.794e-007	3.504e-007	-6.319	-6.455
0.041	KOH	2.912e-014	3.198e-014	-13.536	-13.495
Mg	9.719e-004 Mg+2	8.365e-004	2.512e-004	-3.078	-3.600
-0.522	MgSO4	7.774e-005	8.537e-005	-4.109	-4.069
0.041	MaHCO3+	5.761e-005	4.210e-005	-4.239	-4.376
-0.136	MpCO3	3.967e-008	4.356e-008	-7.402	-7.361
0.041	MbCH+	3.346e-010	2.445e-010	-9.476	-9.612
-0.136 Mp(2)	3 951e-007				
-0.576	Mn+2	2.230e-007	5.922e-008	-6.652	-7.228
_0 136	MnHCO3+	1.035e-007	7.562e-008	-6.985	-7.121
0.136	MnCl+	5.147e-008	3.761e-008	-7.288	-7.425
0.110	Mn904	1.390e-008	1.527e-008	-7.857	-7.816
0.041	MnCl2	2.331e-009	2.560e-009	-8.632	-8.592
0.041	MhCO3	7.786e-010	8.550e-010	-9.109	-9.068
0.041	MnCl3-	1.504e-010	1.099e-010	-9.823	-9.959
-0.136	MnCH+	5.585e-013	4.082e-013	-12.253	-12.389
-0.136 Mn(3)	4.555e-017 Mn+3	4.555e-017	2.710e-018	-16.341	-17.567
-1.220 Na	4.183e-004	4 122- 004	0.051004	2 204	2 520
-0.146	Net	4.1328-004	2.9518-004	-3.304	-3.330
-0.136	NaSO4-	2.934e-006	2.1440-006	-5.533	-5.669
0.041	NahCO3	2.165e-006	2.37/e-006	-5.665	-5.624
-0.136	Nacos-	1.366e-009	9.986e-010	-8.864	-9.001
0.041	NaOH	4.760e-013	5.22/e-013	-12.322	-12.282
O(0)	3.828e-004 02	1.914e-004	2.102e-004	-3.718	-3.677
0.041 S(-2)	0.000e+000				
0.041	H2S	0.000e+000	0.000e+000	-137.957	-137.917
-0.187	HS-	0.000e+000	0.000e+000	-139.239	-139.426
-0.635	S-2	0.000e+000	0.000e+000	-146.277	-146.912
0.041	Fe_di(HS)2	0.000e+000	0.000e+000	-288.693	-288.653
-0.136	Fe_di(HS)3-	0.000e+000	0.000e+000	-425.906	-426.042
S(6)	1.579e-002 CaSO4	9.217e-003	1.012e-002	-2.035	-1.995
0.041	504-2	6.491e-003	1.450e-003	-2.188	-2.839
-0.651	MpSO4	7.774e-005	8.537e-005	-4.109	-4.069
0.041	Na904-	2.934e-006	2.144e-006	-5.533	-5.669
-0.136	H904-	7.130e-007	5.211e-007	-6.147	-6.283
-0.136	K904-	4.794-007	3.504e-007	-6.319	-6.455
-0.136	CaHSO1+	2.999-007	2.192-007	_6 523	-6 650
-0.136	Es trignut	1 5820 000	1 157~ 000	_7 901	פנט.ט דרם ד_
-0.136	MPGU/	1 300- 000	1 5070 000	7 057	7 010
0.041	To try (00110	1.350G-010	1.02/e-008	-1.00/	-/.810
-0.136	re_uri(504)2-	J.UZUE-UIU	3.000E-ULU	-9.299	-9.436
-0.545	re_ur1H904+2	4.013e-013	1.1450-013	10,000	-12.941
0.041	re_cu:su4	4.1/2e-020	4.5828-020	-13.380	-19.339
	re dih904+	1.523e-024	1.113e-024	-23.817	-23 953

I

	Phase	SI log IAP	log KT	
	Anhydrite	0.07 -4.29	-4.36	Ca904
	Aragonite Calcite	0.14 -8.20 0.28 -8.20	-8.34 -8.48	CaCO3
	CH4 (g) -	-138.48 -141.34	-2.86 -1.47	CH4 (1)2
	Dolomite	-1.45 -18.54	-17.09	CaMg(003)2
	H2 (g)	-41.21 -44.36	-3.15	H2
	H2O(g) H2S(g) -	-1.51 -0.00	-1.00	H2O H2S
	Halite Hausmannite	-5.92 -4.34 -8.93 52.10	1.58 61.03	NaCl Mn3O4
	Manganite 02(q)	-1.11 24.23	25.34 -2.89	MnOOH 02
	Pyrochroite Byrolusito	-11.57 3.63	15.20	Mn (CH) 2 Mn C2
	Rhodochrosite	-2.84 -13.97	-11.13	Mh003
Densteinen et er		-101.59 -90.71	4.88	5
MERCULIAN SLEP	)⊥L. vant Do di boa nor	etire mles in	colution	6 750450- 010
WHRIVIING: FIGI	Erroneous mole b	alance occurs a	as moles a	are added to produce
zero moles.	Usually caused h	y KINETICS, REF	CTION, OI	r diffuse layer
calculation.	May be due to la	arge time steps	in early	part of KINEFICS
simulation or WARNING: Elen	r negative concent rent Fe_di has neg Erroneous mole h	rations in the pative moles in palance occurs a	diffuse : solution as moles a	layer. , -4.638259e-020. are added to produce
zero moles.	Usually caused h	y KINETICS, REF	CTION, OI	diffuse layer
calculation.	May be due to la	urge time steos	in earlv	part of KINEFICS
simulation or WARNING: Elem	negative concent rent Fe_di has neg Erroneous mole h	rations in the pative moles in malance occurs a	diffuse : solution as moles a	layer. , -7.131341e-020. are added to produce
zero moles.	Usually caused h	y KINETICS, REF	CTION, 01	: diffuse layer
calculation.	May be due to la	irge time stens	in early	part of KINEFICS
simulation or WARNING: Elen	negative concent rent Fe_di has neg Erroneous mole h	rations in the pative moles in palance occurs a	diffuse solution as moles a	layer. , -5.682284e-020. are added to produce
zero moles.	Usually caused h	y KINETICS, REF	CTION, OI	diffuse layer
calculation.	May be due to la	rge time steps	in early	part of KINETICS
simulation or WARNING: Elen	r negative concent rent Fe_di has neg Erroneous mole h	pations in the pative moles in palance occurs a	diffuse : solution as moles a	layer. , -3.478989e-020. are added to produce
zero moles.	Usually caused h	y KINETICS, REF	CTION, OI	r diffuse layer
calculation.	May be due to la	urge time steps	in early	part of KINETICS
simulation or WARNING: Elen	r negative concent rent Fe_di has neg Erroneous mole h	rations in the pative moles in palance occurs a	diffuse : solution as moles a	layer. , -1.764446e-020. are added to produce
zero moles.	Usually caused k	y KINETICS, REF	CTION, OI	r diffuse layer
calculation. simulation or	May be due to la negative concent	arge time steps crations in the	in early diffuse I	part of KINEFICS layer.
WARNING: Elen	ent Fe_di has neç Erroneous mole h	pative moles in palance occurs a	solution. as moles a	, -8.445617e-022. are added to produce
zero moles.	Usually caused k	y KINETICS, REF	CTION, OI	r diffuse layer
calculation.	May be due to la	rge time steps	in early	part of KINETICS
simulation or Using solution Using pure ph	negative concent n 1. ase assemblage 1.	rations in the	diffuse :	layer.
Using kinetic	15 I. Ki	netics defined	in simula	ition 2.
Kinetics 1.	Kinetics defined	l in simulation	2.	
	Time step: 17280	10 seconds (Inc	remented	time: 864000 seconds)
Coefficient	Rate name	Delta Moles Tot	al Moles	Reactant
1	Fe_di_ax	0.000e+000 9.	.998e-001	Fe_di
1				Fe_tri
T		Dhaco accombla	2000	
		ribbe asseniola	aye	
Delta	Phase	SI log IAP	log KT	'bles in assemblage Initial Final
	02 (a)	-0.78 -3.68	-2.89 1	L.000e+001 1.000e+001
1.243e-013				
		Solution composi	1t1an	
	Elements	Molality	Moles	
	C	1.389e-001 1.	.389e-001	
	CI Po di	2.367e-001 2.	.367e-001	
	Fe_tri	1.610e-004 1.	.055e-022	
	к Mg	5.2/0e-005 5. 9.719e-004 9.	.∠/ue-005 .719e-004	
	Mn Na	3.951e-007 3. 4.183e-004 4.	.951e-007 .183e-004	
	S	1.579e-002 1.	.579e-002	
	De	escription of so	olution	

---Saturation indices--

		pH pe	= 5.432 = 15.170	Charge Adjust	e balance red to redox
equilibrium	Acti I Mass Total alkal Total Total	vity of water anic strength of water (kg) inity (eq/kg) CO2 (mol/kg)	= 0.991 = 4.066e-0 = 1.000e+0 = 2.983e-0 = 1.389e-0	001 000 002 001	
Percent erro	Tempera Electrical or, 100*(Cat- An	ature (deg C) balance (eg)  )/(Cat+ An ) Iterations Total H	= 25.000 = -1.265e-0 = -0.00 = 233 = 1.110421e	)09 >+002	
		Total O	= 5.587731e	+001	
		Distribution c	of species		
				Log	Log
Log	Species	Molality	Activity	Molality	Activity
Gamma		4 504 005	0.000.000	5 200	5 400
-0.113	H+	4.791e-006	3.69/e-006	-5.320	-5.432
-0.187	UH-	4.153e-009	2.0840-009	-8.384	-8.5/1
0.000	0.000-+000	2.2216+001	9.9118-001	1.744	-0.004
0.0/1	CH4	0.000e+000	0.000e+000	-141.384	-141.343
C(4)	1.389e-001	1.094e-001	1.201e-001	-0.961	-0.920
0.041	HCO3-	2.035e-002	1.433e-002	-1.691	-1.844
-0.152	CaHCO3+	9.085e-003	6.396e-003	-2.042	-2.194
-0.152	MgHCO3+	5.761e-005	4.210e-005	-4.239	-4.376
-0.136	CaCO3	9.729e-006	1.068e-005	-5.012	-4.971
0.041	NaHCO3	2.165e-006	2.377e-006	-5.665	-5.624
0.041	003-2	7.400e-007	1.818e-007	-6.131	-6.741
-0.610	MnHCO3+	1.035e-007	7.562e-008	-6.985	-7.121
-0.136	MgCO3	3.967e-008	4.356e-008	-7.402	-7.361
0.041	NaCO3-	1.366e-009	9.986e-010	-8.864	-9.001
-0.136	MhCO3	7.786e-010	8.550e-010	-9.109	-9.068
0.041	Fe_diH003+	9.982e-023	7.295e-023	-22.001	-22.137
-0.136	Fe_diCO3	2.022e-025	2.220e-025	-24.694	-24.654
0.041 Ca	1.476e-001	1 000 001	2 400 000	0.000	1 450
-0.568	Ca+2	1.293e-001	3.499e-002	-0.888	-1.456
0.041	C-1702	9.2170-003	6 2060 002	2.035	-1.995
-0.152	Can.U.S.+	9.0000-000	1 06% 005	-2.042	-2.194
0.041		2 9990 007	2 1020 007	6 523	6 659
-0.136	CaOH+	2 130-009	1 557-009	_8 672	_8 808
-0.136 Cl	2.367e-001	212000 000	1.5570 005	010/2	01000
-0.181	C1-	2.367e-001	1.559e-001	-0.626	-0.807
-0.136	MnCl+	5.147e-008	3.761e-008	-7.288	-7.425
-0.545	Fe_triCl+2	1.201e-008	3.425e-009	-7.921	-8.465
-0.136	Fe_triCl2+	3.264e-009	2.385e-009	-8.486	-8.622
0.041	MnC12	2.331e-009	2.560e-009	-8.632	-8.592
-0.136	MnCl3-	1.504e-010	1.099e-010	-9.823	-9.959
0.041	Fe_triCl3	3.386e-011	3.719e-011	-10.470	-10.430
-0.136	Fe_diCl+	1.500e-023	1.096e-023	-22.824	-22.960
re_ci	3.055e-022 Fe_di+2	1.785e-022	5.092e-023	-21.748	-22.293
-0.545	Fe_diH003+	9.982e-023	7.295e-023	-22.001	-22.137
-0.136	Fe_diCl+	1.500e-023	1.096e-023	-22.824	-22.960
0.011	Fe_diSO4	1.196e-023	1.313e-023	-22.922	-22.882
0.041	Fe_diC03	2.022e-025	2.220e-025	-24.694	-24.654
-0.136	Fe_diOH+	5.908e-027	4.318e-027	-26.229	-26.365
-0.136	Fe_diH904+	4.365e-028	3.190e-028	-27.360	-27.496
0.041	Fe_di(HS)2	0.000e+000	0.000e+000	-292.236	-292.195
-0.136	Fe_di (HS) 3-	0.000e+000	0.000e+000	-429.448	-429.585
Fe_tri	1.610e-004 Fe_tri(OH)2+	1.530e-004	1.118e-004	-3.815	-3.951
-0.136	Fe_triOH+2	4.415e-006	1.259e-006	-5.355	-5.900
-0.545	Fe_tri(OH)3	3.517e-006	3.862e-006	-5.454	-5.413

0.041

-0.136

Fe\_triSO4+

1.583e-008 1.157e-008 -7.801 -7.937

4 005	Fe_tri+3	1.223e-008	7.275e-010	-7.913	-9.138
-1.226	Fe_triCl+2	1.201e-008	3.425e-009	-7.921	-8.465
-0.545	Fe_tri2(OH)2+4	6.446e-009	4.269e-011	-8.191	-10.370
-2.179	Fe_triCl2+	3.264e-009	2.385e-009	-8.486	-8.622
-0.136	Fe tri3(0H)4+5	2.532e-009	9.974e-013	-8.597	-12.001
-3.405	Fe tri (OH) 4-	1.292e-009	9.444e-010	-8.889	-9.025
-0.136	Fe tri (904)2-	5.020e-010	3.668e-010	-9.299	-9.436
-0.136	Fe triCl3	3.386e-011	3.719e-011	-10.470	-10.430
0.041	Fe triH904+2	4 0130-013	1 1/150-013	_12 397	_12 9/1
-0.545	0.0000000	4.0100 010	1.1400 010	12.007	12.941
0.041	H2	0.000e+000	0.000e+000	-44.396	-44.355
K.	5.270e-005	E 222- 00E	3 440- 00F	4 000	4.400
-0.181	K+	5.222e-005	3.4400-005	-4.282	-4.403
-0.136	KS04-	4./94e-00/	3.5040-007	-6.319	-6.455
0.041	KOH	2.912e-014	3.198e-014	-13.536	-13.495
Mg	9.719e-004 Mg+2	8.365e-004	2.512e-004	-3.078	-3.600
-0.522	Mg904	7.774e-005	8.537e-005	-4.109	-4.069
0.041	MgHCO3+	5.761e-005	4.210e-005	-4.239	-4.376
-0.136	MgCO3	3.967e-008	4.356e-008	-7.402	-7.361
0.041	MpCH+	3.346e-010	2.445e-010	-9.476	-9.612
-0.136 Mn(2)	3.951e-007				
-0.576	Mn+2	2.230e-007	5.922e-008	-6.652	-7.228
_0 136	MnHCO3+	1.035e-007	7.562e-008	-6.985	-7.121
0.136	MnCl+	5.147e-008	3.761e-008	-7.288	-7.425
0.041	Mn904	1.390e-008	1.527e-008	-7.857	-7.816
0.041	MnCl2	2.331e-009	2.560e-009	-8.632	-8.592
0.041	MinCO3	7.786e-010	8.550e-010	-9.109	-9.068
0.041	MnCl3-	1.504e-010	1.099e-010	-9.823	-9.959
-0.136	MnCH+	5.585e-013	4.082e-013	-12.253	-12.389
-0.136 Mn(3)	4.555e-017				
-1.226	Mn+3	4.555e-017	2.710e-018	-16.341	-17.567
Na	4.183e-004 Na+	4.132e-004	2.951e-004	-3.384	-3.530
-0.146	Na904-	2.934e-006	2.144e-006	-5.533	-5.669
-0.136	NaHCO3	2.165e-006	2.377e-006	-5.665	-5.624
0.041	NaCO3-	1.366e-009	9.986e-010	-8.864	-9.001
-0.136	NaCH	4.760e-013	5.227e-013	-12.322	-12.282
0.041 O(0)	3.828e-004				
0.041	02	1.914e-004	2.102e-004	-3.718	-3.677
S(-2)	0.000e+000				

0.041	H2S	0.000e+000	0.000e+000	-137.957	-137.917	
0.197	HS-	0.000e+000	0.000e+000	-139.239	-139.426	
0.635	S-2	0.000e+000	0.000e+000	-146.277	-146.912	
-0.035	Fe_di(HS)2	0.000e+000	0.000e+000	-292.236	-292.195	
0.041	Fe <u>di</u> (HS)3-	0.000e+000	0.000e+000	-429.448	-429.585	
-0.156 S(6)	1.579e-002	0.017000	1 010- 000	0.005	1 005	
0.041	Ca504	9.21/e-003	1.012e-002	-2.035	-1.995	
-0.651	504-2	6.491e-003	1.4508-005	-2.188	-2.839	
0.041	Mg904	7.774e-005	8.53/e-005	-4.109	-4.069	
-0.136	NaSO4-	2.934e-006	2.144e-006	-5.533	-5.669	
-0.136	H904-	7.130e-007	5.211e-007	-6.147	-6.283	
-0.136	K904-	4.794e-007	3.504e-007	-6.319	-6.455	
-0.136	CaH904+	2.999e-007	2.192e-007	-6.523	-6.659	
-0.136	Fe_triSO4+	1.583e-008	1.157e-008	-7.801	-7.937	
0.041	MnSO4	1.390e-008	1.527e-008	-7.857	-7.816	
0.041	Fe_tri(SO4)2-	5.020e-010	3.668e-010	-9.299	-9.436	
-0.130	Fe_triH904+2	4.013e-013	1.145e-013	-12.397	-12.941	
-0.545	Fe_di904	1.196e-023	1.313e-023	-22.922	-22.882	
0.041	Fe_diH904+	4.365e-028	3.190e-028	-27.360	-27.496	
-0.136						
		—Saturation i	ndices			
	Phase	SI log I	AP log KT			
	Arhydrite Aragonite Calcite CH(u) CC2(u) Dolomite Oppsun H20(u) H20(u) H20(u) H25(u) Haister Hassentite O2(u) Pyrochosite Pyrolusite Hudodrosite Sulfur	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	CaSO4 CaC03 CaC03 CaM3 CaM5(CO3)2 CaM5(CO3)2 CaSO4:2H2C H2O H2O H2O H2O H2O H2O H2O H2O H2O H2O		
End of simulation.						
Reading input	t data for simula	ation 3.				

End of run.

## **B-3: PHREEQC Partial Output File**

Days	Fe(2)	Fe(3)	pН	si_Fe(OH)3(a)
0.0000e+000	1.6100e+002	0.0000e+000	5.4344e+000	-9.9990e+001
1.1574e-003	1.6023e+002	7.6792e-001	5.4344e+000	-9.9990e+001
5.7870e-003	1.5720e+002	3.7999e+000	5.4344e+000	-9.9990e+001
4.1667e-002	1.3558e+002	2.5417e+001	5.4341e+000	-9.9990e+001
1.6667e-001	8.1085e+001	7.9915e+001	5.4333e+000	-9.9990e+001
4.1667e-001	2.9106e+001	1.3189e+002	5.4326e+000	-9.9990e+001
1.0000e+000	2.6813e+000	1.5832e+002	5.4322e+000	-9.9990e+001
2.0000e+000	4.5311e-002	1.6095e+002	5.4322e+000	-9.9990e+001
4.0000e+000	1.2984e-005	1.6100e+002	5.4322e+000	-9.9990e+001
6.0000e+000	3.7205e-009	1.6100e+002	5.4322e+000	-9.9990e+001
8.0000e+000	1.0661e-012	1.6100e+002	5.4322e+000	-9.9990e+001
1.0000e+001	3.0549e-016	1.6100e+002	5.4322e+000	-9.9990e+001

# Appendix C. Iron Standards Calculations

**Table C-1: Standards Calculations** 

Formula Weight, FeCl3 (g/mol)	270.32
Molar Weight, Fe (g/mol)	55.847
Actual Weight of Compound*, FeCl3 (g)	0.495
Volume of flask (L)	1
Desired Conc. (mg/L)	100
Desired Mass	100
Mass of Compound to produce desired [Fe] (mg)	484.0367

#### Table C-2: Iron Standards

Stand. [C]	Vol.(mL)	Actual Vol (mL)*	Actual Dilution (ppm)
1	0.977852	1	1.02265
2	1.955704	2	2.0453
5	4.88926	5	5.11325
8	7.822816	8	8.1812
50	48.8926	50	51.1325

\*measured quantity