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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

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BRIGHAM YOUNG UNIVERSITY

GRADUATE COMMITTEE APPROVAL

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ABSTRACT

INVESTIGATION OF THE IRON OXIDATION KINETICS IN MANTUA RESERVOIR

Scott H. Lathen

Department of Civil and Environmental Engineering

Master of Science

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 $0.0029 \, \text{min}^{-1}$. 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 $4 \times 10^{13} \, / \, \text{atm} \times \text{min}$.

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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TABLE OF CONTENTS

A	CKN	NOWLEDGMENTS	vii
T	ABLE	E OF CONTENTS	vii
L	IST C	OF TABLES	ix
L	IST O	OF FIGURES	xi
1	Int	ntroduction	1
	1.1	Mantua Reservoir Background	3
	1.2	Objectives	7
2	Ch	hemistry	9
	2.1	Chemical Conditions of Mantua Reservoir	9
	2.2	Iron Oxidation Kinetics	12
	2.3	Factors Affecting Iron Oxidation Kinetics	14
3	Mo	lethods and Experimental Procedures	19
	3.1	Sampling Methods and Locations	19
	3.2	Qualitative Procedures	20
	3.3	DO Testing in Mantua Reservoir	21
	3.4	Laboratory Procedures	23
	3.4	4.1 Anaerobic Conditions	23
	3.4	4.2 Standards	24
	3.4	4.3 Re-aeration and Iron Measurement	26
4	Co	omputer Modeling Procedures	29
	4 1	PHREEOC	29

	4.2	Mantua Model Development	30
5	Exp	perimental and Modeling Results and Discussion	33
	5.1	Field Results	33
	5.2	Qualitative Staining Results	37
	5.3	Quantitative Experimental Results	40
	5.4	PHREEQC Model Results	44
6	Con	ıclusions	49
	6.1	Application	51
Re	eferen	ces	55
Aŗ	pendi	x A. Field Data	57
Aŗ	pendi	x B. PHREEQC Files	59
	B-1: P	artial input file for Example 9 (Parkhurst and Appelo 1999)	59
	B-2: N	Mantua PHREEQC model complete input and output file	61
	B-3: P	HREEQC Partial Output File	78
Δr	nendi	x C. Iron Standards Calculations	79

LIST OF TABLES

Table 1-1: Attributes of Mantua Reservoir	3
Table 2-1: Rate Constants for Iron Oxidation ²	13
Table 3-1: Standards	25
Table 5-1: Staining Observations.	37
Table 5-2: Spectrophotometer Results	41
Table A-1: Field Data Collected from Mantua Reservoir (24 hour period, 9/11/2006).	57
Table C-1: Standards Calculations.	79
Table C-2: Iron Standards	79

LIST OF FIGURES

Figure 1-1: Headstone staining (Wood 2002)	2
Figure 1-2 : Mantua reservoir	4
Figure 2-1: March 31st results (Wallace 2006)	11
Figure 3-1: Aerial view of Mantua Reservoir	20
Figure 3-2: Iron standards calibration curve	26
Figure 5-1: DO and temp measurements	34
Figure 5-2: Concrete before spraying	38
Figure 5-3: Stained concrete	39
Figure 5-4: Iron oxidation over time	42
Figure 5-5: Revised iron oxidation over time	43
Figure 5-6: Change in iron concentration using default <i>k</i>	44
Figure 5-7: Model vs experimental iron concentrations	46
Figure 5-8: Model of Mantua iron oxidation kinetics	46

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 (Fe³⁺) 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).

Table 1-1: Attributes of Mantua Reservoir

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).

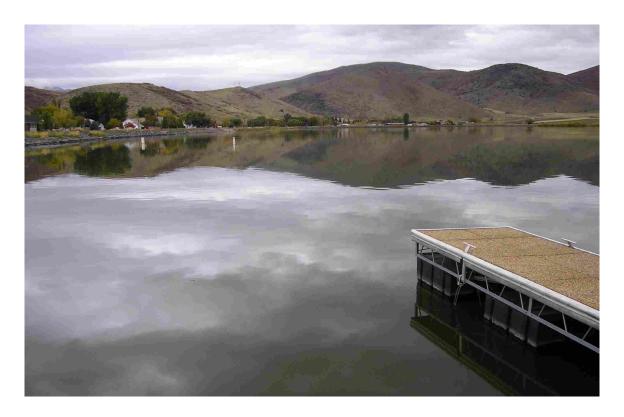


Figure 1-2: Mantua Reservoir

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 18th and August 10th 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 μg/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 18th, when low DO

levels were measured farther from the reservoir bottom. On July 18th 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 (Fe²⁺) 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.

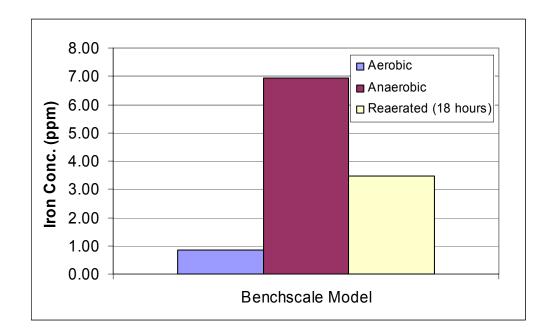


Figure 2-1: March 31st results (Wallace 2006)

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 (Fe³⁺) 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.

Table 2-1: Rate Constants for Iron Oxidation²

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

¹rate constant for concentration of dissolved oxygen

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)

² Modified from Houben (2004)

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 1.0×10^{-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).

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

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 Cu²⁺ and Co²⁺ 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 Fe²⁺ onto ferric oxide and the rate constant of the oxidation at the surface. The value of this constant is given as 1.71×10^{-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 10⁶ (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 Fe²⁺ 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 8th, 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 8th, 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 8th, 2006 (the day the probe was deployed) were run on October 21st, 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 31st, 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 (FeCl₃) 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.

Table 3-1: Standards

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

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.

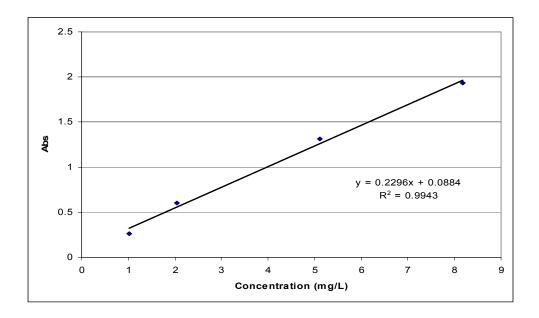


Figure 3-2: Iron standards calibration curve

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 Fe²⁺ to Fe³⁺ in water (Parkhurst and Appelo 1999). The rate equation, Equation 4-1, used in the model was adapted from Singer and Stumm (1970):

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

where t equals the time in seconds, a^2_{OH} 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 11th, 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

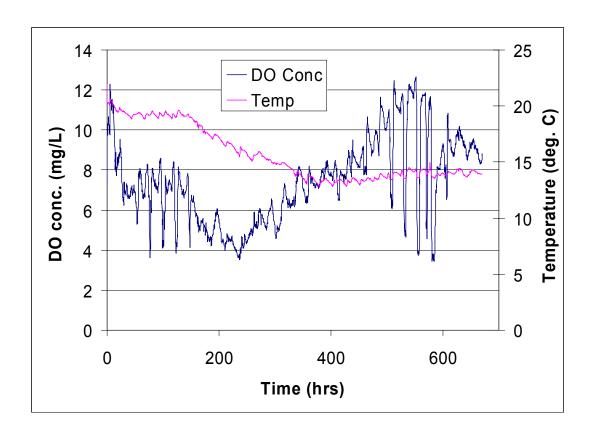


Figure 5-1: DO and temp measurements

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).

$$K_H = \frac{P_{gas}}{C_{equ}} \tag{5.1}$$

 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-m³/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/m³ 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.

Table 5-1: Staining Observations

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

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.

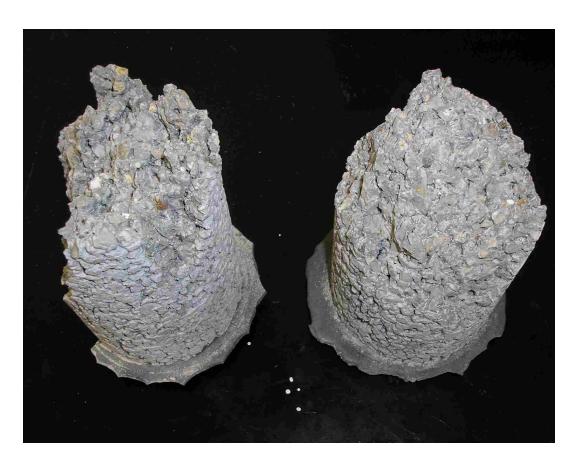


Figure 5-2: Concrete before spraying



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

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.

Table 5-2: Spectrophotometer Results

Date	Sample	Time Removed	Run Time	ΔT (min)	abs	[Fe] mg/L	Average [Fe] 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	

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.

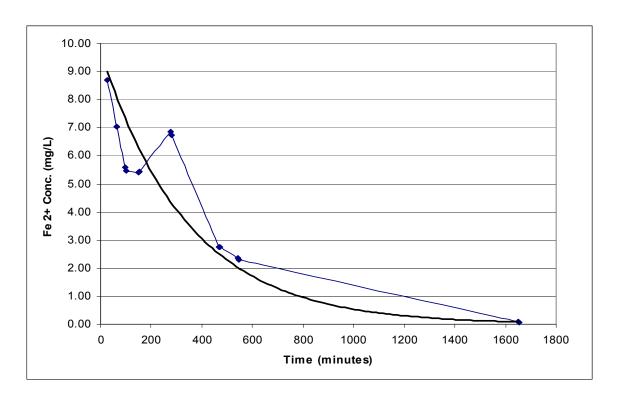


Figure 5-4: Iron oxidation over time

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.

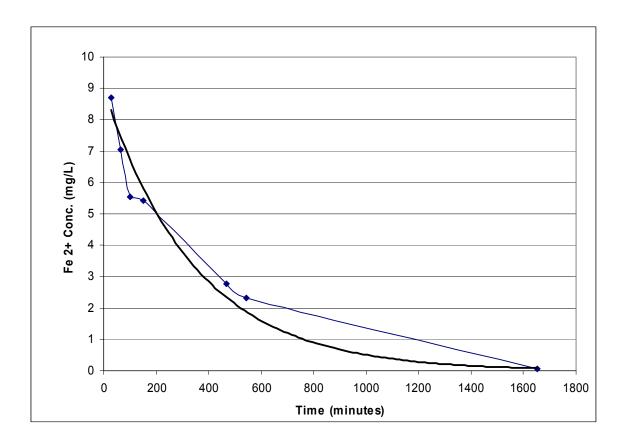


Figure 5-5: Revised iron oxidation over time

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:

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

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⁻¹, 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 (Fe²⁺) and ferric iron (Fe³⁺) versus time. Figure 5-6 is the plot produced using the default rate constant.

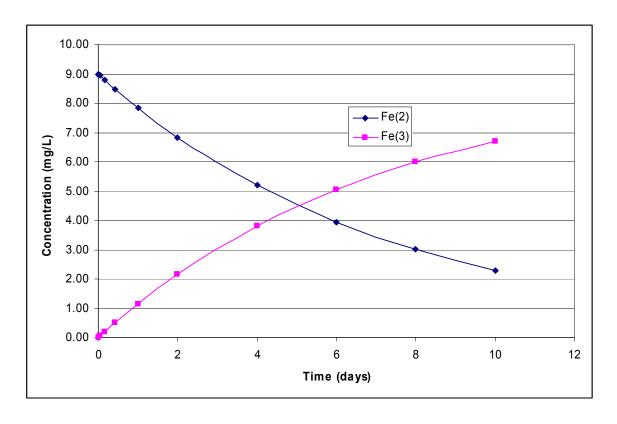


Figure 5-6: Change in iron concentration using default k

As the ferric iron concentration rises, due to the solubility product being extremely low (K_{sp} = 2.79x10⁻³⁹), 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 $4x10^{13}$ /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

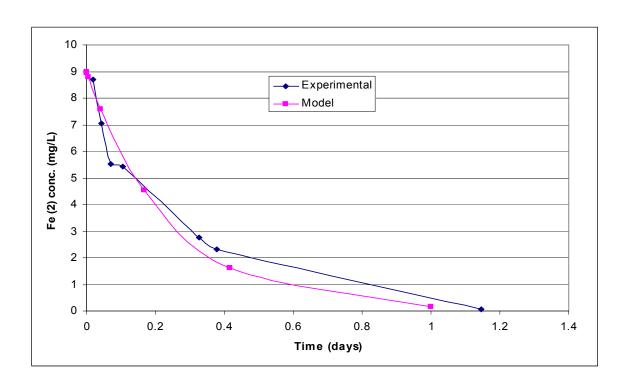


Figure 5-7: Model vs experimental iron concentrations

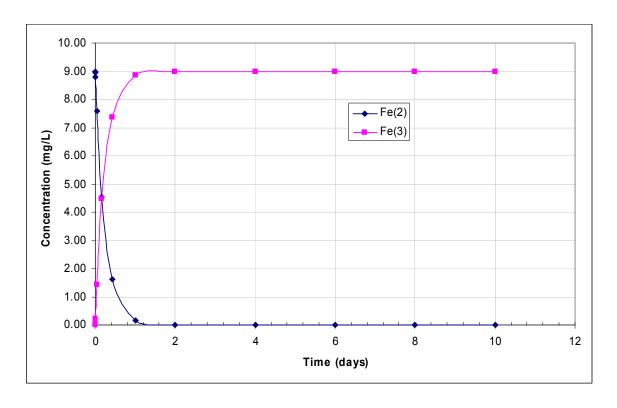


Figure 5-8: Model of Mantua iron oxidation kinetics

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 10⁶ (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⁻¹, 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)

DateTime M/D/Y	Temp C	ODO Conc (mg/L)	Resistivity KOhm.cm	TDS g/L	Salinity ppt	SpCond mS/cm	ODO% %
9/11/2006 0:00	19.39	7.97	5.83	0.125	0.09	0.192	86.7
9/11/2006 0:00	19.38	8.07	5.84	0.125	0.09	0.192	87.7
9/11/2006 0:13	19.38	7.93	5.84	0.125	0.09	0.192	86.2
9/11/2006 0:30	19.36	7.86	5.84	0.125	0.09	0.192	85.4
9/11/2006 0:45	19.37	7.81	5.84	0.125	0.09	0.192	84.9
			5.6 4 5.84				86.1
9/11/2006 1:15	19.37	7.93		0.125	0.09	0.192	
9/11/2006 1:30	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 2:00	19.29	7.75	5.85	0.125	0.09	0.192	84
9/11/2006 2:15	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	80.3
9/11/2006 2:45	19.22	7.3	5.85	0.125	0.09	0.192	79.1
9/11/2006 3:00	19.21	7.33	5.85	0.125	0.09	0.192	79.4
9/11/2006 3:15	19.19	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	75.5
9/11/2006 3:45	19.14	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	74.7
9/11/2006 4:30	19.12	6.96	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 5:00	19.02	6.66	5.87	0.125	0.09	0.192	71.8
9/11/2006 5:15	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	72.1
9/11/2006 5:45	19	6.77	5.87	0.125	0.09	0.193	73
9/11/2006 6:00	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 6:30	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	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	72.6
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 8:45	18.84	6.64	5.9	0.125	0.09	0.192	71.4
9/11/2006 9:00	18.86	6.95	5.9	0.125	0.09	0.192	74.7
9/11/2006 9:05	18.91	7.05	5.9	0.125	0.09	0.192	75.9
9/11/2006 9:13	18.88	7.18	5.9	0.125	0.09	0.192	77.3
9/11/2006 9:35	18.94	7.10	5.89	0.125	0.09	0.192	78.7
9/11/2006 9.45	19.94	7.45	5.89	0.125	0.09	0.192	80.3
		7.45 7.7			0.09		83.2
9/11/2006 10:15	19.09		5.87	0.125		0.192	
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 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
	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
#
# 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
\#\dots and also other Fe+3 species
PHASES
Goethite
         Fe_{tri00H} + 3 H + = Fe_{tri} + 3 + 2 H20
         log_k -1.0
SOLUTION 1
         рH 7.0
         pe 10.0 O2(g) -0.67
         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_o2 = 10^(SI("02(g)"))
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:\Thesis\Kinetics17.pqi
                                                                                                                                                                                                                                                                                                                                                                                                 Example 9.—Kinetically controlled oxidation of ferrous iron. Decoupled valence states of iron.
  Output file: F:\Thesis\Kinetics17.pgp
Database file: E:\Program Files\WX3\Phreeqc Interactive 2.12.5\phreeqc.dat
  Reading data base.
                                                                                                                                                                                                                                                                                                                                                                                               End of simulation.
                                                           SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
                                                                                                                                                                                                                                                                                                                                                                                                Reading input data for simulation 2.
                                                             HASES
EXCHANGE_MASTER_SPECTES
EXCHANGE_SPECTES
SURFACE_MASTER_SPECTES
SURFACE_SPECTES
SURFACE_SPECTES
                                                                                                                                                                                                                                                                                                                                                                                                                                                        SOLUTION 1
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        N 1
pH 4.535
pe -0.924 C2(g) -0.785
Fe_di 0.161
Na 0.4183
C1 0.3216 charge
                                                             RATES
END
  Reading input data for simulation 1.
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          Mg 0.9719
Mn 0.0003951
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          Ca 147.6
Alkalinity 29.67
C 138.9
S 15.79
                                                          DATABASE E:\Program Files\USGS\Phreeqc Interactive
EQUILIBRIUM PHASES 1
02 (g)
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             -0.785
                                                                                                                                                                                                                                                                                                                                                                                                                                                       RATES
Fe_di_ox
                                                    Fe_tri Fe_tri+3 0.0 Fe_tri

SILUTION_SHCIES
Fe_di+2 = Fe_di+2 | log_k 0.0
Fe_tri+3 = Fe_tri+3 | log_k 0.0
Fe_tri+3 = Fe_tri+3 | log_k 0.0
Fe_di+2 + H20 = Fe_diGH+ H+ | log_k -9.5 | delta_h 13.20 kcal Fe_di+2 + G3-2 = Fe_diGG+ | log_k 0.14
Fe_di+2 + G3-2 = Fe_diGG+ | log_k 0.14
Fe_di+2 + G3-2 = Fe_diGG+ | log_k 0.14
Fe_di+2 + H38 = Fe_diHO3+ | log_k 2.05 | kcal Fe_di+2 + H38 = Fe_diHO3+ | log_k 2.05 | kcal Fe_di+2 + H394 = Fe_diHO3+ | log_k 2.05 | kcal Fe_di+2 + H394 = Fe_diHO3+ | log_k 2.05 | kcal Fe_di+2 + H394 = Fe_diHFO4+ | log_k 2.05 | kcal Fe_di+2 + H394 = Fe_diHFO4+ | log_k 2.05 | kcal Fe_di+2 + H394 = Fe_diHFO4+ | log_k 2.05 | kcal Fe_di+2 + H394 = Fe_diHFO4+ | log_k 2.05 | kcal Fe_di+2 + H394 = Fe_diHFO4+ | log_k 2.05 | kcal Fe_di+3 + H394 = Fe_diHFO4+ | log_k 2.05 | kcal Fe_di+3 + H394 = Fe_diHFO4+ | log_k 2.05 | kcal Fe_di+3 + H394 = Fe_diHFO4+ | log_k 2.05 | kcal Fe_di+3 + H394 = Fe_diHFO4+ | log_k 2.05 | kcal Fe_di+3 + H394 = Fe_diHFO4+ | log_k 2.05 | kcal Fe_di+3 + H394 = Fe_diHFO4+ | log_k 2.05 | kcal Fe_di+3 + H394 = Fe_diHFO4+ | log_k 2.05 | kcal Fe_di+3 + H394 = Fe_diHFO4+ | log_k 2.05 | kcal Fe_di+3 + H394 = Fe_diHFO4+ | log_k 2.05 | kcal Fe_di+3 + H394 = Fe_diHFO4+ | log_k 2.05 | kcal Fe_di+3 + H394 = Fe_diHFO4+ | log_k 2.05 | kcal Fe_di+3 + H394 = Fe_diHFO4+ | log_k 2.05 | kcal Fe_di+3 + H394 = Fe_diHFO4+ | log_k 2.05 | kcal Fe_di+3 + H394 = Fe_diHFO4+ | log_k 2.05 | kcal Fe_di+3 + H394 = Fe_diHFO4+ | log_k 2.05 | kcal Fe_di+3 + H394 = Fe_diHFO4+ | log_k 2.05 | kcal Fe_di+3 + H394 = Fe_diHFO4+ | log_k 2.05 | kcal Fe_di+3 + H394 = Fe_diHFO4+ | log_k 2.05 | kcal Fe_di+3 + H394 = Fe_diHFO4+ | log_k 2.05 | kcal Fe_di+3 + H394 = Fe_diHFO4+ | log_k 2.05 | kcal Fe_di+3 + H394 = Fe_diHFO4+ | log_k 2.05 | kcal Fe_di+3 + H394 = Fe_diHFO4+ | log_k 2.05 | kcal Fe_di+3 + H394 = Fe_diHFO4+ | log_k 2.05 | kcal Fe_di+3 + H394 = Fe_diHFO4+ | log_k 2.05 | kcal Fe_di+3 + H394 = Fe_diHFO4+ | log_k 2.05 | kcal Fe_di+3 + H394 = Fe_diHFO4+ | log_k 2.05 | kcal Fe_di+3 + H394 = Fe_diHFO4+ | log_k 2.05 | kcal Fe_di+3
                                                          Fe_tri
                                                                                                                                           Fe_tri+3 0.0
                                                                                                                                                                                                                         Fe_tri
  55.847
                                                                                                                                                                                                                                                                                                                                                                                                                                                       returo.

start. di = TOT("Fe_di")

20 if (Fe_di <= 0) then goto 200

30 p.o2 = 10"(ST ("O2(g)"))

40 mbles = (2.91e-9 + 4e1) * (ACT("OH-"))"2 * p.o2) * Fe_di *
                                                             SOLUTION_SPECIES
                                                                                                                                                                                                                                                                                                                                                                                             TIME
                                                                                                                                                                                                                                                                                                                                                                                                                                                        200 SAVE moles
                                                                                                                                                                                                                                                                                                                                                                                         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.
                                                                                                                                                                                                                                                                                                                                                                                                                                                         KINETICS 1
                                                                                                                                                                                                                                                                                                                                                                                             Beginning of initial solution calculations.
                                                                                                                                                                                                                                                                                                                                                                                             Initial solution 1.
                                                                                                                                                                                                                                                                                                                                                                                             pH will be adjusted to obtain desired alkalinity.
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             ----Solution composition-
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       Molality
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               2.967e-002 2.967e-002
1.389e-001 1.389e-001
1.476e-001 1.476e-001
2.367e-001 2.367e-001
                                                                                                                                                                                                                                                                                                                                                                                                                                                        Alkalinity
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    Charge balance
                                                                                                                                                                                                                                                                                                                                                                                                                                                       Fe_di
K
Mg
Mn
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 1.610e-004
5.270e-005
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  1.610e-004
5.270e-005
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                9.719e-004
3.951e-007
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  9.719e-004
3.951e-007
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                4.183e-004 4.183e-004
1.579e-002 1.579e-002
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   -Description of solution-
                                                                                                                                                                                                                                                                                                                                                                                            O2 (g)
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   Activity of water
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         Ionic strength
Mass of water (kg)
Total CO2 (mol/kg)
Temperature (deg C)
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                4.068e-001
1.000e+000
                                                        log k 1.13

Fe tri+3 + 504-2 = Fe tri+504+
log k 4.04
delta h 3.91 kcal

Fe tri+3 + H504- = Fe tri+504+2
log k 2.48

Fe tri+3 + 2504-2 = Fe tri+504+2
log k 5.38
delta h 3.60 kcal

Fe tri+3 + HF04- = Fe tri+HF04+
log k 5.43
delta h 5.76 kcal

Fe tri+3 + H2F04 = Fe tri+HF04+2
log k 5.43
Fe tri+3 + H2F04 = Fe tri+HF04+2
log k 5.43
Fe tri+3 + 2 F = Fe tri+2
log k 6.2
delta h 2.7 kcal

Fe tri+3 + 2 F = Fe tri+2+1
log k 10.8
delta h 3.8 kcal

Fe tri+3 + 3 F = Fe tri+5
log k 14.0
delta h 5.4 kcal

Fe tri+3 + 3 F = Fe tri+5
log k 14.0
delta h 5.4 kcal

Fe tri+3 + 3 F = Fe tri+5
log k 14.0
delta h 5.4 kcal

Fe tri+3 + 3 F = Fe tri+5
log k 14.0
delta h 5.4 kcal
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                1.389e-001
25.000
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 = 25.000
= -3.112e-015
= -0.00
= 19
= 1.110421e+002
= 5.587722e+001
                                                                                                                                                                                                                                                                                                                                                                                                 Electrical balance (eq)
Percent error, 100*(Cat-|An|)/(Cat+|An|)
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                Iterations
Total H
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   -Distribution of species
                                                                                                                                                                                                                                                                                                                                                                                            Log
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       Molality Activity Molality Activity
                                                                                                                                                                                                                                                                                                                                                                                            Gamma
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                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
                                                                                                                                                                                                                                                                                                                                                                                                                                                            1.389e-001
```

	002	1.092e-001	1.200e-001	-0.962	-0.921
0.041	H003-	2.043e-002	1.438e-002	-1.690	-1.842
-0.152	CaH003+	9.116e-003	6.417e-003	-2.040	-2.193
-0.152	MgHCO3+	5.781e-005	4.225e-005	-4.238	-4.374
-0.136	Fe_diH003+	5.274e-005	3.854e-005	-4.278	-4.414
-0.136	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	1.834e-007	-6.127	-6.737
-0.610	Fe_diCO3	1.074e-007	1.179e-007	-6.969	-6.928
0.041	MnHCO3+	1.037e-007	7.582e-008	-6.984	-7.120
-0.136	MgCCC3	4.001e-008	4.394e-008	-7.398	-7.357
0.041	Nacco3-	1.378e-009	1.007e-009	-8.861	-8.997
-0.136	MnCO3	7.846e-010	8.617e-010	-9.105	-9.065
0.041 Ca	1.476e-001	1.293e-001	3.498e-002	-0.889	-1.456
-0.568	Ca+2				
0.041	CaSO4 CaHOO3+	9.212e-003 9.116e-003	1.012e-002 6.417e-003	-2.036 -2.040	-1.995 -2.193
-0.152	CaCO3	9.811e-006	1.077e-005	-5.008	-2.193 -4.968
0.041	CaUS CaH9O4+	2.982e-007	2.180e-007	-6.525	-6.662
-0.136	CC2201				
-0.136 Cl	CaOH+ 2.367e-001	2.141e-009	1.565e-009	-8.669	-8.806
-0.181	Cl-	2.367e-001	1.559e-001	-0.626	-0.807
-0.136	Fe_diCl+	7.893e-006	5.768e-006	-5.103	-5.239
-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
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_dis04	6.292e-006	6.909e-006	-5.201	-5.161
0.041	Fe_diCO3	1.074e-007	1.179e-007	-6.969	-6.928
0.041	Fe_diOH+	3.126e-009	2.284e-009	-8.505	-8.641
-0.136	Fe_diHSO4+	2.285e-010	1.670e-010	-9.641	-9.777
-0.136	Fe_di.(HS)2	0.000e+000	0.000e+000	-274.519	-274.479
0.041	Fe_di(HS)3-	0.000e+000	0.000e+000	-411.734	-411.870
-0.136 H(0)					
11(0)	0.000e+000	0.000000	0.000-+000		
0.041	H2	0.000e+000	0.000e+000	-44.396	-44.355
0.041 K		0.000e+000 5.222e-005	0.000e+000 3.439e-005		
0.041 K -0.181	H2 5.270e-005			-44.396	-44.355
0.041 K -0.181 -0.136	H2 5.270e-005 K+	5.222e-005	3.439e-005	-44.396 -4.282	-44.355 -4.464
0.041 K -0.181	H2 5.270e-005 K+ KSO4- KOH 9.719e-004	5.222e-005 4.793e-007 2.927e-014	3.439e-005 3.503e-007 3.214e-014	-44.396 -4.282 -6.319 -13.534	-44.355 -4.464 -6.456 -13.493
0.041 K -0.181 -0.136 0.041	H2 5.270e-005 K+ KS04- KCH 9.719e-004 Mg+2	5.222e-005 4.793e-007 2.927e-014 8.364e-004	3.439e-005 3.503e-007 3.214e-014 2.511e-004	-44.396 -4.282 -6.319 -13.534 -3.078	-44.355 -4.464 -6.456 -13.493 -3.600
0.041 K -0.181 -0.136 0.041	H2 5.270e-005 K+ K504- KCH 9.719e-004 Mg+2 Mg504	5.222e-005 4.793e-007 2.927e-014 8.364e-004 7.770e-005	3.439e-005 3.503e-007 3.214e-014 2.511e-004 8.532e-005	-44.396 -4.282 -6.319 -13.534 -3.078 -4.110	-44.355 -4.464 -6.456 -13.493 -3.600 -4.069
0.041 K -0.181 -0.136 0.041 Mg -0.523	H2 5.270e-005 K+ KS04- KCH 9.719e-004 Mg+2 MgS04 MgH003+	5.222e-005 4.793e-007 2.927e-014 8.364e-004	3.439e-005 3.503e-007 3.214e-014 2.511e-004 8.532e-005 4.225e-005	-44.396 -4.282 -6.319 -13.534 -3.078	-44.355 -4.464 -6.456 -13.493 -3.600
0.041 K -0.181 -0.136 0.041 Mg -0.523 0.041	H2 5.270e-005 K+ K504- KCH 9.719e-004 Mg+2 Mg504	5.222e-005 4.793e-007 2.927e-014 8.364e-004 7.770e-005 5.781e-005 4.001e-008	3.439e-005 3.503e-007 3.214e-014 2.511e-004 8.532e-005 4.225e-005 4.394e-008	-44.396 -4.282 -6.319 -13.534 -3.078 -4.110 -4.238	-44.355 -4.464 -6.456 -13.493 -3.600 -4.069 -4.374
0.041 K -0.181 -0.136 0.041 Mg -0.523 0.041 -0.136	H2 5.270e-005 K+ KS04- KCH 9.719e-004 Mg+2 MgS04 MgHC03+ MgC03	5.222e-005 4.793e-007 2.927e-014 8.364e-004 7.770e-005 5.781e-005	3.439e-005 3.503e-007 3.214e-014 2.511e-004 8.532e-005 4.225e-005 4.394e-008 2.457e-010	-44.396 -4.282 -6.319 -13.534 -3.078 -4.110 -4.238 -7.398	-44.355 -4.464 -6.456 -13.493 -3.600 -4.069 -4.374 -7.357
0.041 K -0.181 -0.136 0.041 Mg -0.523 0.041 -0.136 0.041 -0.136	H2 5.270e-005 K+ KS04- KCH 9.719e-004 Mg+2 Mg504 MgH003+ Mg003 Mg0H+	5.222e-005 4.793e-007 2.927e-014 8.364e-004 7.770e-005 5.781e-005 4.001e-008	3.439e-005 3.503e-007 3.214e-014 2.511e-004 8.532e-005 4.225e-005 4.394e-008	-44.396 -4.282 -6.319 -13.534 -3.078 -4.110 -4.238 -7.398	-44.355 -4.464 -6.456 -13.493 -3.600 -4.069 -4.374 -7.357
0.041 K -0.181 -0.136 0.041 Mg -0.523 0.041 -0.136 0.041 -0.136 Mn(2)	H2 5.270e-005 K+ KS04- KCH 9.719e-004 Mg+2 MgS04 MgH003+ MgC03 MgCH+ 3.951e-007 Mn+2 MrH003+	5.222e-005 4.793e-007 2.927e-014 8.364e-004 7.770e-005 5.781e-005 4.001e-008 3.362e-010 2.228e-007 1.037e-007	3.439e-005 3.503e-007 3.214e-014 2.511e-004 8.532e-005 4.225e-005 4.394e-008 2.457e-010 5.916e-008 7.582e-008	-44.396 -4.282 -6.319 -13.534 -3.078 -4.110 -4.238 -7.398 -9.473 -6.652 -6.984	-44.355 -4.464 -6.456 -13.493 -3.600 -4.069 -4.374 -7.357 -9.610 -7.228 -7.120
0.041 K -0.181 -0.136 0.041 Mg -0.523 0.041 -0.136 0.041 -0.136 Mn(2) -0.576	H2 5.270e-005 K+ KS04- KCH 9.719e-004 Mg+2 MgS04 MgH003+ MgC03 MgCH+ 3.951e-007 Mn+2 MrH003+	5.222e-005 4.793e-007 2.927e-014 8.364e-004 7.770e-005 5.781e-005 4.001e-008 3.362e-010 2.228e-007 1.037e-007 5.141e-008	3.439e-005 3.503e-007 3.214e-014 2.511e-004 8.532e-005 4.225e-005 4.394e-008 2.457e-010 5.916e-008 7.582e-008 3.757e-008	-44.396 -4.282 -6.319 -13.534 -3.078 -4.110 -4.238 -7.398 -9.473 -6.652 -6.984 -7.289	-44.355 -4.464 -6.456 -13.493 -3.600 -4.069 -4.374 -7.357 -9.610 -7.228 -7.120 -7.425
0.041 K -0.181 -0.136 0.041 Mg -0.523 0.041 -0.136 0.041 -0.136 Nn(2) -0.576 -0.136	H2 5.270e-005 K+ KS04- KS19-004 Mg+2 Mg504 MgH003+ MgC03 MgCH+ 3.951e-007 Mh+2 MH003+ MrCl+ MrS04	5.222e-005 4.793e-007 2.927e-014 8.364e-004 7.770e-005 5.781e-005 4.001e-008 3.362e-010 2.228e-007 1.037e-007 5.141e-008 1.389e-008	3.439e-005 3.503e-007 3.214e-014 2.511e-004 8.532e-005 4.225e-005 4.394e-008 2.457e-010 5.916e-008 7.582e-008 3.757e-008	-44.396 -4.282 -6.319 -13.534 -3.078 -4.110 -4.238 -7.398 -9.473 -6.652 -6.994 -7.289 -7.857	-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
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	H2 5.270e-005 K+ KS04- KSH 9.719e-004 Mg+2 Mg504 MgH003+ MgC03 MgCH+ 3.951e-007 Mr+2 MrH003+ MrC12	5.222e-005 4.793e-007 2.927e-014 8.364e-004 7.770e-005 5.781e-005 4.001e-008 3.362e-010 2.228e-007 1.037e-007 5.141e-008 1.389e-008 2.328e-009	3.439e-005 3.503e-007 3.214e-014 2.511e-004 8.532e-005 4.225e-005 4.394e-008 2.457e-010 5.916e-008 3.757e-008 1.525e-008 2.557e-009	-44.396 -4.282 -6.319 -13.534 -3.078 -4.110 -4.238 -7.398 -9.473 -6.652 -6.994 -7.289 -7.857 -8.633	-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
0.041 K -0.181 -0.136 0.041 Mg -0.523 0.041 -0.136 0.041 -0.136 -0.136 -0.136 -0.136 0.041	H2 5.270e-005 K+ KS04- KSH 9.719e-004 Mg+2 Mg504 MgH003+ MgC03 MgCH+ 3.951e-007 Mr+2 MrH003+ MrC12 MrC12 MrC03	5.222e-005 4.793e-007 2.927e-014 8.364e-004 7.770e-005 5.781e-005 4.001e-008 3.362e-010 2.228e-007 1.037e-007 5.141e-008 1.389e-008 2.328e-009 7.846e-010	3.439e-005 3.503e-007 3.214e-014 2.511e-004 8.532e-005 4.225e-005 4.394e-008 2.457e-010 5.916e-008 7.582e-008 3.757e-008 1.525e-009 8.617e-010	-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	-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
0.041 K -0.181 -0.136 0.041 Mg -0.523 0.041 -0.136 0.041 -0.136 -0.136 -0.136 -0.136 0.041 0.041	H2 5.270e-005 K+ KS04- KCH 9.719e-004 MgH2 MgS04 MgH03+ MgC03 MgCH+ 3.951e-007 Mh12 MH108+ MHC1+ MHS04 MHC12 MHC03 MHC13-	5.222e-005 4.793e-007 2.927e-014 8.364e-004 7.770e-005 5.781e-005 4.001e-008 3.362e-010 2.228e-007 1.037e-007 5.141e-008 1.389e-008 2.328e-009 7.846e-010 1.502e-010	3.439e-005 3.503e-007 3.214e-014 2.511e-004 8.532e-005 4.225e-005 4.394e-008 2.457e-010 5.916e-008 7.582e-008 3.757e-008 1.525e-008 2.557e-009 8.617e-010 1.098e-010	-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	-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 -9.960
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	H2 5.270e-005 K+ KS04- KCH 9.719e-004 MgH28 MgS04 MgH03+ MgC03 MgCH+ 3.951e-007 Mh+2 MrH03+ MrC1+ MrS04 MrC12 MrC03 MrC13- MrCH+	5.222e-005 4.793e-007 2.927e-014 8.364e-004 7.770e-005 5.781e-005 4.001e-008 3.362e-010 2.228e-007 1.037e-007 5.141e-008 1.389e-008 2.328e-009 7.846e-010	3.439e-005 3.503e-007 3.214e-014 2.511e-004 8.532e-005 4.225e-005 4.394e-008 2.457e-010 5.916e-008 7.582e-008 3.757e-008 1.525e-009 8.617e-010	-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	-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
0.041 K -0.181 -0.136 0.041 Mg -0.523 0.041 -0.136 0.041 -0.136 -0.136 -0.136 0.041 0.041 0.041 0.041 -0.136 -0.136 Mn(3)	H2 5.270e-005 K+ KS04- KCH 9.719e-004 MgH2 MgS04 MgH03+ MgC03 MgCH+ 3.951e-007 Mh12 MH108+ MHC1+ MHS04 MHC12 MHC03 MHC13-	5.222e-005 4.793e-007 2.927e-014 8.364e-004 7.770e-005 5.781e-005 4.001e-008 3.362e-010 2.228e-007 1.037e-007 5.141e-008 1.389e-008 2.328e-009 7.846e-010 1.502e-010	3.439e-005 3.503e-007 3.214e-014 2.511e-004 8.532e-005 4.225e-005 4.394e-008 2.457e-010 5.916e-008 7.582e-008 3.757e-008 1.525e-008 2.557e-009 8.617e-010 1.098e-010	-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	-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 -9.960
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	H2 5.270e-005 K+ KS04- KCH 9.719e-004 Mg+2 Mg504 Mg403+ Mg003 Mg0H+ 3.951e-007 Mn+2 MrH003+ MrC1+ MrS04 MrC12 Mr003 MrC13- MrC13- MrC13- MrC14 4.528e-017 Mn+3 4.183e-004	5.222e-005 4.793e-007 2.927e-014 8.364e-004 7.770e-005 5.781e-005 4.001e-008 3.362e-010 2.228e-007 1.037e-007 5.141e-008 1.389e-008 2.328e-009 7.846e-010 1.502e-010 5.608e-013	3.439e-005 3.503e-007 3.214e-014 2.511e-004 8.532e-005 4.225e-005 4.394e-008 2.457e-010 5.916e-008 7.582e-008 3.757e-008 6.15257e-009 8.617e-010 4.098e-013 2.693e-018	-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	-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 -9.960 -12.387 -17.570
0.041 K -0.181 -0.136 0.041 Mg -0.523 0.041 -0.136 0.041 -0.136 Nh(2) -0.576 -0.136 -0.041 0.041 0.041 0.041 0.041 -0.136 0.041 -0.136 -0.136	H2 5.270e-005 K+ KS04- KCH 9.719e-004 Mg+2 Mg604 Mg403+ Mg03 Mg0H+ 3.951e-007 Mn+2 MrH003+ MrC1+ MrS04 MrC12 Mr03 MrC13- MrC13- MrC13- MrC13- MrC13- MrC14 MrS04 MrC14 MrC14 MrS04 MrC12 MrC13-	5.222e-005 4.793e-007 2.927e-014 8.364e-004 7.770e-005 5.781e-005 4.001e-008 3.362e-010 2.228e-007 1.037e-007 5.141e-008 1.389e-008 2.328e-009 7.846e-010 1.502e-010 5.608e-013 4.528e-017	3.439e-005 3.503e-007 3.214e-014 2.511e-004 8.532e-005 4.225e-005 4.394e-008 2.457e-010 5.916e-008 7.582e-008 3.757e-008 1.525e-008 4.098e-010 4.098e-013 2.693e-018	-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	-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 -9.960 -12.387 -17.570 -3.530
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 0.041 0.041 0.041 0.041 0.041 0.041 0.041 0.041 0.041	H2 5.270e-005 K+ KS04- KCH 9.719e-004 Mg+2 Mg604 Mg403+ Mg603 Mg0H+ 3.951e-007 Mn+2 Mr103+ MrC12 Mr603 MrC13- Mr0H+ 4.528e-017 Mr+3 4.183e-004 Na+ Na604-	5.222e-005 4.793e-007 2.927e-014 8.364e-004 7.770e-005 5.781e-005 4.001e-008 3.362e-010 2.228e-007 5.141e-008 1.389e-008 2.328e-009 7.846e-010 1.502e-010 5.608e-013 4.528e-017 4.132e-004 2.933e-006	3.439e-005 3.503e-007 3.214e-014 2.511e-004 8.532e-005 4.225e-005 4.394e-008 2.457e-010 5.916e-008 7.582e-008 3.757e-008 1.525e-008 4.098e-010 4.098e-013 2.693e-018 2.950e-004 2.143e-006	-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	-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 -9.960 -12.387 -17.570 -3.530 -5.669
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 -0.136 -0.136 Na -0.136 Na -0.136 Na	H2 5.270e-005 K+ KS04- KCH 9.719e-004 Mg+2 Mgs04 MgH03+ MgG03 MgGH+ 3.951e-007 Mn+2 MH003+ MH003+ MHC1+ MH003+ MHC12 MH003 MHC12 MH004 MHC12 MH003 MHC13- MH0H 4.528e-017 Mn+3 4.183e-004 NRH NRS04- NRH003	5.222e-005 4.793e-007 2.927e-014 8.364e-004 7.770e-005 5.781e-005 4.001e-008 3.362e-010 2.228e-007 1.037e-007 5.141e-008 1.389e-008 2.328e-009 7.846e-010 1.502e-010 5.608e-013 4.528e-017 4.132e-004 2.933e-006 2.172e-006	3.439e-005 3.503e-007 3.214e-014 2.511e-004 8.532e-005 4.225e-005 4.394e-008 2.457e-010 5.916e-008 7.582e-008 3.757e-008 1.525e-008 4.098e-010 4.098e-013 2.693e-018 2.950e-004 2.143e-006 2.386e-006	-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 -5.663	-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 -9.960 -12.387 -17.570 -3.530 -5.669 -5.622
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 -0.136 -0.136 Na -0.146 -0.146 -0.136	H2 5.270e-005 K+ KS04- KCH 9.719e-004 Mg+2 Mg604 Mg403+ Mg603 Mg0H+ 3.951e-007 Mn+2 Mr103+ MrC12 Mr603 MrC13- Mr0H+ 4.528e-017 Mr+3 4.183e-004 Na+ Na604-	5.222e-005 4.793e-007 2.927e-014 8.364e-004 7.770e-005 5.781e-005 4.001e-008 3.362e-010 2.228e-007 5.141e-008 1.389e-008 2.328e-009 7.846e-010 1.502e-010 5.608e-013 4.528e-017 4.132e-004 2.933e-006	3.439e-005 3.503e-007 3.214e-014 2.511e-004 8.532e-005 4.225e-005 4.394e-008 2.457e-010 5.916e-008 7.582e-008 3.757e-008 1.525e-008 4.098e-010 4.098e-013 2.693e-018 2.950e-004 2.143e-006	-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	-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 -9.960 -12.387 -17.570 -3.530 -5.669

0.041	NaOH	4.784e-013	5.253e-013	-12.320	-12.280
O(0)	3.828e-004 02	1.914e-004 2	2.102e-004	-3.718	-3.677
0.041 S(-2)	0.000e+000 H2S	0.000e+000 (0000=+000	_137_962	_137 921
0.041	HS-		0.000e+000		
-0.187	S-2		0.000e+000		
-0.635	Fe_di(HS)2	0.000e+000 (0.000e+000	-274.519	-274.479
0.041	Fe_di(HS)3-	0.000e+000 (0.000e+000	-411.734	-411.870
-0.136 S(6)	1.579e-002 CaSO4	9.212e-003 1	1 012=-002	-2.036	-1.995
0.041	SO4-2	6.490e-003			-2.839
-0.651	MgSO4		3.532e-005		-4.069
0.041	Fe_dis04	6.292e-006 6	5.909e-006		-5.161
0.041	NaSO4-	2.933e-006 2	2.143e-006	-5.533	-5.669
-0.136	H904-	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	CaH904+	2.982e-007 2	2.180e-007	-6.525	-6.662
-0.136	MnSO4	1.389e-008 1	1.525e-008	-7.857	-7.817
0.041	Fe_diH904+	2.285e-010 1	1.670e-010	-9.641	-9.777
-0.136		Saturation in	diana		
		Sacuracion in			
	Phase	SI log IAI	P log KT		
	Arhydrite Aragonite Calcite CH(g) CU2(g) Dolomite Gypsun H2(g) H20(g) H20(g) H31ite Hausmanite Hausmanite C1(g) Pyrodroite Pyrolusite Rhododrosite Sulfur	0.07 4.2 0.14 -8.1; 0.29 -8.1; -138.48 -141.3; 0.55 -0.28 -4.3; -1.41 -18.5; -1.21 -44.3; -1.51 -0.0; -1.59.2 -137.9; -1.59.2 -137.9; -1.59.2 -13.6; -1.57 -3.6; -1.57 -3.6; -1.57 -3.6; -1.57 -3.6; -1.51 -0.0; -1.0, 0.0; -1.0, 0.0	9 -8.34 -8.48 4 -2.86 2 -1.47 -17.09 -4.58 5 -3.15 1.51 2 -1.00 1.58 1 61.03 4 25.34 25.34 41.38 -2.89 3 -15.15 -11.13	CaCO3 CaCO3 CH4 CD2 CaMg(CO3))2 CaMg(CO3))2 CaSO4:2H2O H2 H2O H2S MaC1 Mn3O4 MnOCH O2 Mn(CH)2	
Reaction ste	_				
Using pure p Using kineti	hase assemblage	1. Kinetics defined	d in simula	ation 2.	
Kinetics 1.	Kinetics defin	ned in simulation	n 2.		
	Time step: 10	seconds (Incre	emented ti	me: 100 sec	ands)
Obefficient	Rate name	Delta Moles To	otal Moles	Reactant	
	Fe_di_ax	-7.679e-007 1	1.000e+000	Fe_di	
-1				Fe_tri	
1					
		Phase assemb	Lage		
	M	OT 1 TN	D 3 700	Moles in as	semblage
Delta	Phase	SI log IAI	P 10g KI	Initial	Final
1.920e-007	O2 (g)	-0.78 -3.68	3 -2.89	1.000e+001	1.000e+001-
		Solution compo	sition		
	Elements	Molality	Moles		
	C Ca Cl Fe_di Fe_tri K Mg Mn	1.476e-001 1 2.367e-001 2 1.602e-004 1 7.679e-007 5 5.270e-005 9 9.719e-004 9 3.951e-007 3	1.389e-001 1.476e-001 2.367e-001 1.602e-004 7.679e-007 5.270e-005 9.719e-004 3.951e-007 4.183e-004		
	Na S	4.183e-004 4 1.579e-002 1	1.579e-002		
	Na S	1.579e-002 1 -Description of s	1.579e-002		
equilibrium	Na S	1.579e-002 1	1.579e-002 solution = 5.434 = 15.168 = 0.991 = 4.068e-	Adjust	:balance ed to redox

Total alkalinity (eq/kg) = 2.967e-002
Total CO2 (mol/kg) = 1.389e-001
Temperature (eg/ c) = 25.000
Electrical balance (eg) = -1.008e-014
Percent error, 100*(Cat-|kn|)/(Cat-|kn|) = -0.00
Ilerations = 4
Total H = 1.110421e+002
Total O = 5.587722e+001

-Distribution of species-Log Log Log Species Molality Activity Molality Activity H+ 4.767e-006 3.678e-006 -5.322 -5.434 -0.113 4.154e-009 2.698e-009 -8.382 OH--8.569 -0.187 5.551e+001 9.911e-001 H2O 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-001 002 1.092e-001 1.200e-001 -0.962 -0.921 0.041 H003-2.043e-002 1.438e-002 -1.690 -1.842 -0.152 CaH003+ 9.116e-003 6.417e-003 -2.040 -2.193 -0.152 MgHC03+ 5.781e-005 4.225e-005 -4.238 -4.374 -0.136 Fe_diH003+ 5.249e-005 3.836e-005 -4.280 -0.136 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 -6.127 CC3-2 7.466e-007 1.833e-007 -6.737 -0.610 Fe_di003 1.068e-007 1.173e-007 -6.971 -6.931 0.041 MnH003+ 1.037e-007 7.582e-008 -6.984 -7.120 -0.136 MgC03 4.001e-008 4.393e-008 -7.398 -7.357 0.041 Nacco3-1.378e-009 1.007e-009 -8.861 -8.997 -0.136 MnCO3 7.846e-010 8.617e-010 -9.105 -9.065 0.041 Ca 1.476e-001 Ca+2 1.293e-001 3.498e-002 -0.889 -1.456 -0.568 Ca904 9.212e-003 1.012e-002 -2.036 -1.995 0.041 CaHOO3+ 9.116e-003 6.417e-003 -2 040 -2 193 -0.152 CaCO3 9.811e-006 1.077e-005 -5.008 -4.968 0.041 CaHSO4+ 2.982e-007 2.180e-007 -6.525 -6.662 -0.136 CaCH+ 2.141e-009 1.564e-009 -8.669 -8.806 -0.136 Cl 2.367e-001 Cl-2.367e-001 1.559e-001 -0.626 -0.807 -0.181 Fe diCl+ 7.855e-006 5.741e-006 -5.105 -5.241 -0.136 MnC1+ 5.141e-008 3.757e-008 -7.289 -7.425 -0.136 MnC12 2.328e-009 2.557e-009 -8 633 -8 592 0.041 MnC13-1.502e-010 1.098e-010 -9.823 -9.960 -0.136 Fe_triCl+2 5.669e-011 1.617e-011 -10.246 -10.791 -0.545 Fe_triCl2+ 1.541e-011 1.126e-011 -10.812 -10.948 -0.136 Fe_triCl3 1.599e-013 1.756e-013 0.041 1.602e-004 Fe_di+2 Fe di 9.352e-005 2.668e-005 -4.029 -4.574 -0.545 Fe_diH003+ 5.249e-005 3.836e-005 -4.280 -4.416 -0.136 Fe diCl+ 7.855e-006 5.741e-006 -5.105 -5.241 -0.136 Fe di:904 6.262e-006 6.876e-006 -5.203 -5.163 0.041 Fe_dicc3 1.068e-007 1.173e-007 -6.971 -6.931 0.041 Fe_diOH+ 3.111e-009 2.274e-009 -8.507 -8.643 -0.136 Fe_diH904+ 2.275e-010 1.662e-010 -9.643 -9.779 -0.136 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 7.679e-007 Fe_tri 7.299e-007 5.334e-007 -6.137 Fe_tri(OH)2+ -6.273 -0.136 Fe_triOH+2 2.095e-008 5.978e-009 -7.679 -8.223 -0.545Fe_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_triCl+2 5.669e-011 1.617e-011 -10.246 -0.545 Fe_triCl2+ 1.541e-011 1.126e-011 -10.812 -10.948 -0.136 6.228e-012 4.551e-012 -11.206 -11.342 Fe_tri(OH)4-

-0.136

0.041	Dharv						
0.041		e	STloot	AP log KT			
-2.179 Fe_trisO(H)2+4			-Saturation i	ndices			
-2.179 Fe_tris(CH)2+4	Fe_t:	riHSO4+2	1.885e-015	5.377e-016	-14.725	-15.26	9
0.041						-11.76	
-0.041 -2.179 -0.545 -0.545 -0.545 -0.545 -0.545 -0.545 -0.545 -0.545 -0.545 -0.545 -0.545 -0.545 -0.000e+000 -0.001 -0.136 -0	_					-10.26	
0.041						-9.77	
0.041						-7.81	
0.041	CaH90	24 +				-6.66	
-0.041 -2.179 -0.545 -3.405 -3						-6.45	
-0.041 -2.179 -0.545 -3.405 -3						-6.28	
-0.041 -2.179 -0.545 -3.405 -3						-5.669	
-0.041 -2.179 -2.179 -0.545 -3.405 -3.405 -3.405 -3.406 -3						-5.16	
-0.041 -2.179 -2.179 -0.545 -0.545 -0.545 -0.006+000 -0.006+000 -0.006+000 -0.006+000 -0.006+000 -0.006+000 -0.006+000 -0.006+000 -0.006+000 -0.006+000 -0.006+000 -0.006+000 -0.011 -0.136 -0.1379=-000 -0.000+000 -0.0	_		7.770e-005	8.532e-005	-4.110	-4.069	9
-0.041 -2.179 -0.545 -0.545 -0.545 -0.545 -0.000e+000 -0.000e+000 -0.001 -0.041 -0.000e+000 -0.000e+000 -0.001 -0.041 -0.136 -0.1378-000 -0.000+000 -0	S04-2	2	6.490e-003	1.449e-003	-2.188	-2.83	9
-0.041 -2.179 -2.179 -0.545 -0.545 -0.545 -0.006+000 -0.006+000 -0.006+000 -0.006+000 -0.006+000 -0.006+000 -0.011 -0.136			9.212e-003	1.012e-002	-2.036	-1.99	5
-0.041 -2.179 -0.545 -0.545 -0.545 -0.000e+000 -0.000e+000 -0.001 -0.001 -0.001 -0.001 -0.001 -0.001 -0.001 -0.001 -0.136	_		0.000e+000	0.000e+000	-4TT*/20	- 411. 8/	_
-0.041 -2.179 -0.545 -0.545 -0.545 -0.000e+000 -0.000e+000 -0.01 -0.01 -0.01 -0.136 -0.136 -0.041 -0.136 -0						-274.48 -411.87	
-0.041 -2.179 -0.545 -0.545 -0.545 -0.000e+000 -0.001 -0.041 -0.000e+000 -0.001 -0.018 -0.136 -0.13798-009		- (ma) -				-146.912	
-0.041 -2.179 -0.545 -0.545 -0.545 -0.000e+000 -0.001 -0.041 -0.000e+000 -0.001 -0.041 -0.136						-139.42	
-0.041 -2.179 -0.545 -0.545 -0.545 -0.545 -0.00e+000 -0.00e+000 -0.00e+000 -0.011 -0.041 -0.136 -0.1						-137.92	
-0.041 -2.179 -0.545 -0.545 -0.545 -0.545 -0.000e+000 -0.001 -0.001 -0.001 -0.001 -0.001 -0.001 -0.001 -0.001 -0.0136 -0.0136 -0.030 -0.030 -0.031 -0.032 -0.0336 -0.034 -0.034 -0.136 -		000e+000					
-0.041 -2.179 -0.545 -0.545 -0.545 -0.545 -0.545 -0.000e+000 -0.018 -0.136 -0.13		828e-004	1.914e-004	2.102e-004	-3.718	-3.67	7
0.041 -2.179 -0.545 Fe_triHS04+2 1.885e-015 5.377e-016 -14.725 -15 Fe_triHS04+2 1.885e-015 1.072e-019 -15.565 -18 Fe_triHS04+2 1.085e-016 1.072e-019 -15.565 -18 Fe_triHS04+2 1.085e-016 1.072e-019 -15.565 -18 Fe_triHS04+2 1.000e+000 0.000e+000 0.000e+000 -44.396 -46 -46 -47 -47 -47 -47 -47 -47 -47 -47 -47 -47			4.784e-013	5.253e-013	-12.320	-12.28	0
0.041 -2.179 -0.545 Fe_triHS04+2 1.885e-015 5.377e-016 -14.725 -15 Fe_triHS04+2 1.885e-015 1.072e-019 -15.565 -18 Fe_triHS04+2 1.000e+000 0.000e+000 0.000e+000 -44.396 -46 -46 -47 -48 -483e-004 -48.38e-005 -48 -48 -483e-005 -48 -48 -483e-006 -48 -483e-006 -48 -483e-006 -48 -48 -483e-006 -48 -483e-006 -48 -483e-006 -48 -48 -483e-006 -48 -483e-006 -48 -48 -483e-006 -48 -483e-006 -13.534 -13 -13 -13 -13 -13 -13 -13 -13 -13 -13			1.378e-009	1.007e-009		-8.99	
-0.041 -2.179 -0.545 -0.545 -0.545 -0.545 -0.546 -0.546 -0.545 -0.546 -0.546 -0.546 -0.547 -0.547 -0.548 -0.6000 -0.00000000						-5.62	
0.041 -2.179 -0.545 -0.545 -0.545 -0.545 -0.000e+000 -0.001 -0.000000 -0.000-		4–				-5.66	
-0.041 -2.179 -0.545 -0.545 -0.545 -0.545 -0.545 -0.000e+000 -0.001 -0.041 -0.136 -0.1		183e-004	4.132e-004	2.950e-004	-3.384	-3.530	0
0.041 -2.179 -0.545 -0.545 -0.545 -0.545 -0.545 -0.000e+000 -0.001 -0.001 -0.001 -0.001 -0.001 -0.001 -0.001 -0.0136 -0.041 -0.136 -0.136 -0.041 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.041 -0.136 -0.041 -0.136 -0.136 -0.041 -0.136 -0.136 -0.041 -0.136 -0.041 -0.136 -0.041 -0.136 -0.041 -0.136 -0.041 -0.136 -0.041 -0.136 -0.041 -0.136 -0.041 -0.0	Mn+3		4.528e-017	2.693e-018	-16.344	-17.570	0
0.041 -2.179 -0.545 -0.545 -0.545 -0.545 -0.545 -0.545 -0.000000000 0.001 -0.0000000000			5.6UKE-U13	4.098E-013	-1∠.251	-12.38	1
0.041 -2.179 -0.545 -0.545 -0.545 -0.545 -0.545 -0.00000000000000000000000000000000000						-9.96	
0.041 -2.179 -0.545 -0.545 -0.545 -0.545 -0.545 -0.545 -0.000000000 -0.00000000 -0.00000000 -0.001 -0.136 -			7.0100 010			-9.06	
0.041 -2.179 Fe_tri2(CH)2+4 1.452e-013 9.618e-016 -12.838 -15 Fe_triBOH+2 1.885e-015 5.377e-016 -14.725 -15 -16 -14.725 -15 -16 -16 -16 -17 -18 -18 -17 -18 -18 -18 -18 -18 -18 -18 -18 -18 -18		_				-8.592	
0.041 -2.179 -0.545 -0.545 -0.545 -0.545 -0.545 -0.545 -0.545 -0.545 -0.545 -0.545 -0.545 -0.545 -0.545 -0.545 -0.545 -0.545 -0.0000000 -0.0000000 -0.001 -0.001 -0.001 -0.001 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.041 -0.136 -0.136 -0.041 -0.136 -0.041 -0.136 -0.041 -0.136 -0.041 -0.136 -0.041 -0.523 -0.041 -0.136 -0.041 -0	Mnso	4	1.389e-008			-7.81	
0.041 -2.179 Fe_tri2(CH)2+4 1.452e-013 9.618e-016 -12.838 -15 Fe_triBOM+2 1.885e-015 5.377e-016 -14.725 -15 -15 -15 -15 -15 -15 -15 -15 -15 -1	MhCl-	+	5.141e-008	3.757e-008	-7.289	-7.42	5
0.041 -2.179 Fe_tri2(CH)2+4 1.452e-013 9.618e-016 -12.838 -15 Fe_tri3(CH)2+5 1.885e-015 5.377e-016 -14.725 -15 -15 -15 -15 -15 -15 -15 -15 -15 -1	MhHO	O3+	1.037e-007	7.582e-008	-6.984	-7.12	.0
0.041 -2.179 Fe_tri2(CH)2+4 1.452e-013 9.618e-016 -12.838 -15 Fe_tri3(CH)2+5 1.885e-015 5.377e-016 -14.725 -15 -15 -15 -15 -15 -15 -15 -15 -15 -1			2.228e-007	5.916e-008	-6.652	-7.22	8
0.041 -2.179 -0.545 -0.545 -0.545 -0.545 -0.545 -0.00000000000000000000000000000000000	_		3.362e-010	2.457e-010	-9.473	-9.61	U
0.041 -2.179 Fe_tri2(CH)2+4 1.452e-013 9.618e-016 -12.838 -15 -15 -15 -15 -15 -15 -15 -15 -15 -15						-7.35	
0.041 -2.179 Fe_tri2(CH)2+4 1.452e-013 9.618e-016 -12.838 -15 -15 -15 -15 -15 -15 -15 -15 -15 -15	_					-4.37	
0.041 -2.179 -0.545 -0.545 -0.545 -0.545 -0.545 -0.545 -0.545 -0.545 -0.545 -0.545 -0.545 -0.545 -0.545 -0.545 -0.545 -0.545 -0.545 -0.000000000 -0.0000000 -0.0000000 -0.0000000 -0.0000000 -0.00000000	MgSO	4	7.770e-005	8.532e-005	-4.110	-4.06	9
0.041 -2.179 -0.545 -0.545 -3.405 H(0) -0.000e+000 -0.181 -0.136 -0.136 -0.136 -0.136 -0.136 -0.137 -0.136 -0.041 -2.179 -0.2179 -0.545 -0.180 -0.000e+000 -0.000e			8.364e-004		-3.078	-3.60	0
0.041 -2.179 -0.545 -0.545 -3.405 H(0) -0.000e+000 -0.041 K -0.181 -0.136 -0.136 -0.139 -0.13		719e-004	2.72/E-U14	J.214C-U14	-10.004	-13.49	
0.041 -2.179 Fe_tri2(CH)2+4 1.452e-013 9.618e-016 -12.838 -15 -15 -15 -15 -15 -15 -15 -15 -15 -15		-					
0.041 -2.179 Fe_tri2(CH)2+4 1.452e-013 9.618e-016 -12.838 -15 -15 -15 -15 -15 -15 -15 -15 -15 -15						-4.46 -6.45	
0.041 -2.179 Fe_tri2(CH)2+4 1.452e-013 9.618e-016 -12.838 -15 -15 -15 -15 -15 -15 -15 -15 -15 -15		270e-005	F 000 00=	2 420 05=	4 000		
-2.179 Fe_tri2(CH)2+4 1.452e-013 9.618e-016 -12.838 -15 -2.179 Fe_triHSO4+2 1.885e-015 5.377e-016 -14.725 -15 -0.545 Fe_tri3(CH)4+5 2.721e-016 1.072e-019 -15.565 -18		000e+000	0.000e+000	0.000e+000	-44.396	-44.35	5
0.041 Fe_tri2(OH)2+4 1.452e-013 9.618e-016 -12.838 -15 Fe_triHSO4+2 1.885e-015 5.377e-016 -14.725 -15	Fe_t:	ri3 (OH) 4+5	2.721e-016	1.072e-019	-15.565	-18.970	0
0.041 Fe_tri2(OH)2+4 1.452e-013 9.618e-016 -12.838 -15	Fe_t:	riH904+2	1.885e-015	5.377e-016	-14.725	-15.26	9
Fe_triCl3 1.599e-013 1.756e-013 -12.796 -12	Fe_t:	ri2(OH)2+4	1.452e-013	9.618e-016		-15.01	7
-0.136	Fe_t:	riCl3	1.599e-013	1.756e-013	-12.796	-12.75	6
	Fe_t:	ri (SO4) 2-	2.369e-012	1.731e-012	-11.625	-11.76	2

 Presse
 SI log IAP
 log KT

 Aragunite
 0.07
 -4.29
 -4.36
 Ca004

 Aragunite
 0.14
 -8.19
 -8.34
 Ca003

 CH4(g)
 -18.48
 -141.34
 -2.86
 CH4

 CU2(g)
 0.55
 -0.92
 -1.47
 CU2

 Dolomite
 -1.44
 -18.53
 -17.09
 Cabg(03)2

 Gypsum
 0.28
 -4.30
 -4.58
 Ca00:2420

 H2(g)
 -41.21
 -44.36
 -3.15
 H2

 H20(g)
 -1.51
 -20.00
 1.51
 H20

 H2S(g)
 -136.92
 -137.92
 -1.00
 H2S

	Halite Hausmannite	-5.92 -4. -8.92 52.	34 1.58 1 11 61.03			0.041	CaSO4	9.212e-003	1.012e-002	-2.036	-1.995
	Manganite	-1.10 24. -0.78 -3.	24 25.34	Mh00H		-0.152	CaH003+	9.115e-003	6.417e-003	-2.040	-2.193
	02(g) Pyrochroite	-11.57 3.	63 15.20	Min (OH)2		0.041	CaCO3	9.809e-006	1.077e-005	-5.008	-4.968
	Pyrolusite Rhodochrosite Sulfur	3.46 44. -2.83 -13. -101.60 -96.	96 -11.13	MinCO3		-0.136	CaHSO4+	2.983e-007	2.180e-007	-6.525	-6.662
Reaction ste		-101.00 -90.	/2 4.00	5		-0.136	CaOH+	2.140e-009	1.564e-009	-8.669	-8.806
Using solution						CI -0.130	2.367e-001 Cl-	2 3670 001	1.559e-001	-0.626	-0.807
	hase assemblage	1. Kinetics defin	ed in cimila	tion 2		-0.181	Fe_diCl+		5.632e-006	-5.113	-5.249
Kinetics 1.				ciui z.		-0.136	MnCl+		3.757e-008	-7.289	-7.425
14120100 11	Time step: 400			e - 500 sec	nnds)	-0.136	MhCl2		2.557e-009	-8.633	-8.592
	Rate name	Delta Moles				0.041	Fe_triCl+2		8.005e-011	-9.552	-10.097
Coefficient						-0.545	MhCl3-		1.098e-010	-9.823	-9.959
-1	Fe_di_ax	-3.032e-006	1.000e+000	Fe_di		-0.136	Fe_triCl2+		5.574e-011	-10.118	-10.254
1				Fe_tri		-0.136	Fe_triCl3		8.689e-013	-12.102	-12.061
		Phase assen	ıblage			0.041 - Fe_di	1.572e-004				
						-0.545	Fe_di+2	9.175e-005	2.617e-005	-4.037	-4.582
	Phase	SI log I	AP log KT	bles in as Initial	ssemblage Final	-0.136	Fe_diH003+	5.149e-005	3.763e-005	-4.288	-4.424
Delta						-0.136	Fe_diCl+		5.632e-006	-5.113	-5.249
7.581e-007	O2 (g)	-0.79 -3.	68 –2.89 1	.000e+001	1.000e+001-	0.041	Fe_di:904		6.746e-006	-5.212	-5.171
		-Solution comp	osition			- 0.041	Fe_diCO3		1.151e-007	-6.980	-6.939
						-0.136	Fe_diOH+		2.230e-009	-8.515	-8.652
	Elements	Molality	Moles			-0.136	Fe_diH904+		1.631e-010	-9.651	-9.788
	C Ca	1.389e-001 1.476e-001	1.476e-001			0.041	Fe_di.(HS)2		0.000e+000	-274.530	-274.489
	Cl Fe_di	2.367e-001 1.572e-004	1.572e-004			-0.136	Fe_di.(HS)3-	0.000e+000	0.000e+000	-411.744	-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 Mn		3.951e-007			-0.136	Fe_triOH+2	1.037e-007	2.958e-008	-6.984	-7.529
	Na S	1.579e-002	4.183e-004 1.579e-002			-0.545 0.041	Fe_tri(OH)3	8.344e-008	9.163e-008	-7.079	-7.038
		Description of	solution			-0.136	Fe_triSO4+	3.698e-010	2.702e-010	-9.432	-9.568
		rU.	= 5.434	Charre	e balance	-1.226	Fe_tri+3	2.859e-010	1.700e-011	-9.544	-10.769
equilibrium			= 15.168		ted to redox		Fe_triCl+2	2.806e-010	8.005e-011	-9.552	-10.097
CQUITIZION.	Acti T	vity of water onic strength	= 0.991 = 4.068e-0	101		-0.136	Fe_triCl2+	7.627e-011	5.574e-011	-10.118	-10.254
	Mass	of water (kg) inity (eq/kg)	= 1.000e+0 = 2.967e-0	100		-0.136	Fe_tri(OH)4-	3.081e-011	2.252e-011	-10.511	-10.647
	Total	CO2 (mol/kg) ature (deg C)	= 1.389e-0 = 25.000	01		-0.136	Fe_tri(SO4)2-	1.173e-011	8.569e-012	-10.931	-11.067
Pement em		balance (eg)	= 2.518e-0	14		-2.179	Fe_tri2(OH)2+4	3.556e-012	2.355e-014	-11.449	-13.628
	, (Iterations		+002		0.041	Fe_triCl3	7.912e-013	8.689e-013	-12.102	-12.061
			= 5.587723e			-3.405	Fe_tri3(OH)4+5	3.297e-014	1.299e-017	-13.482	-16.886
		Distribution o	of species-			-0.545	Fe_triHSO4+2	9.330e-015	2.662e-015	-14.030	-14.575
				Log	Log	H(0)	0.000e+000 H2	0.000e+000	0.000e+000	-44.396	-44.355
Log	Species	Molality	Activity	Molality	Activity	0.041 K	5.270e-005				
Gamma.						-0.181	K+		3.439e-005	-4.282	-4.464
-0.113	H+		3.678e-006	-5.322	-5.434	-0.136	K904-		3.503e-007	-6.319	-6.456
-0.187	OH-		2.698e-009	-8.382	-8.569	0.041	KOH	2.926e-014	3.214e-014	-13.534	-13.493
0.000	H2O	2.55Te+00T	9.911e-001	1.744	-0.004	Mg	9.719e-004 Mg+2	8.364e-004	2.511e-004	-3.078	-3.600
C(-4) 0.041	0.000e+000 CH4	0.000e+000	0.000e+000	-141.384	-141.344	-0.523 0.041	MgSO4	7.770e-005	8.533e-005	-4.110	-4.069
C(4)	1.389e-001 002	1.092e-001	1 2005 001	-0.962	-0.921	-0.136	MgHCO3+	5.780e-005	4.225e-005	-4.238	-4.374
0.041	H003-		1.438e-002	-1.690	-1.842	0.041	MgCO3	4.000e-008	4.393e-008	-7.398	-7.357
-0.152	CaHCO3+		6.417e-003	-2.040	-2.193	-0.136	MgCH+	3.362e-010	2.457e-010	-9.473	-9.610
-0.152	MgHC03+		4.225e-005	-4.238	-4.374	Mn(2)	3.951e-007 Mn+2	2.228e-007	5.917e-008	-6.652	-7.228
-0.136	Fe_diH003+		3.763e-005	-4.288	-4.424	-0.576	MnHCO3+		7.581e-008	-6.984	-7.120
-0.136	CaCO3		1.077e-005	-5.008	-4.968	-0.136	MnCl+		3.757e-008	-7.289	-7.425
0.041	NaHCO3		2.385e-006	-5.663	-5.622	-0.136	MnSO4		1.525e-008	-7.857	-7.817
0.041	003-2		1.833e-007	-6.127	-6.737	0.041	MnCl2		2.557e-009	-8.633	-8.592
-0.610	Fe_diCO3	1.048e-007		-6.980	-6.939	0.041	MnCO3		8.615e-010	-9.105	-9.065
0.041	MnHC03+		7.581e-008	-6.984	-7.120	0.041	MnCl3-		1.098e-010	-9.823	-9.959
-0.136	MgCO3		4.393e-008	-7.398	-7.357	-0.136	MnCH+		4.098e-013	-12.251	-12.387
0.041	NaCO3-	1.378e-009	1.007e-009	-8.861	-8.997	-0.136 Mn(3)	4.528e-017		0.655		
-0.136	Mncc3	7.845e-010	8.615e-010	-9.105	-9.065	-1.226	Mn+3	4.528e-017	2.693e-018	-16.344	-17.570
0.041 Ca	1.476e-001	1 202 201	3 400 000	0.000	1 450	Na 0.146	4.183e-004 Na+	4.132e-004	2.950e-004	-3.384	-3.530
-0.568	Ca+2	1.293e-001	3.498e-002	-0.889	-1.456	-0.146	Na:904-	2.933e-006	2.143e-006	-5.533	-5.669
						-0.136					

Using soluti	on 1. hase assemblage 1	inetics defined in similation 2.
Reaction ste		101.00 30.72 4.00 5
	Manganite 02(g) Pyrochroite Pyrolusite Rhodochrosite Sulfur	-1.10 24.24 25.34 MrOOH -0.79 -3.68 -2.89 02 -11.57 3.63 15.20 Mr(CH)2 3.46 44.84 41.38 MrO2 -2.83 -13.96 -11.13 MrOOB -101.60 -96.72 4.88 S
	H2O(g) H2S(g) Halite Hausmannite	-136.92 -137.92 -1.00 H2S -5.92 -4.34 1.58 NaCl -8.92 52.11 61.03 Mn3O4
	Dolamite Gypsum H2(g) H2O(a)	-1.44 -18.53 -17.09 CaVg(CO3)2 0.28 -4.30 -4.58 CaSO4:2H2O -41.21 -44.36 -3.15 H2 -1.51 -0.00 1.51 H2O
	Aragonite Calcite CH4(g) CC2(g)	0.14 -8.19 -8.34 CaCO3 0.29 -8.19 -8.48 CaCO3 -138.48 -141.34 -2.86 Ct4 0.55 -0.92 -1.47 CC2
	Phase Anhydrite	SI log IAP log KT 0.07 -4.29 -4.36 CaSO4
-0.545 		-Saturation indices
-0.136	Fe_tri(SO4)2- Fe_triHSO4+2	1.173e-011 8.569e-012 -10.931 -11.06 9.330e-015 2.662e-015 -14.030 -14.57
-0.136	Fe_diH904+	2.232e-010 1.631e-010 -9.651 -9.78 1.173e-011 8.569e-012 -10.931 -11.06
-0.136	Fe_triSO4+	3.698e-010 2.702e-010 -9.432 -9.56
0.130	Mn904	1.389e-008 1.525e-008 -7.857 -7.81
-0.136 -0.136	CaHSO4+	2.983e-007 2.180e-007 -6.525 -6.66
-0.136 0.136	K904-	4.793e-007 3.503e-007 -6.319 -6.45
-0.136	H904-	7.092e-007 5.183e-007 -6.149 -6.28
0.041	NaSO4-	2.933e-006 2.143e-006 -5.533 -5.66
0.041	MgSO4 Fe_diSO4	7.770e-005 8.533e-005 -4.110 -4.06 6.143e-006 6.746e-006 -5.212 -5.17
-0.651	SO4-2	6.490e-003 1.449e-003 -2.188 -2.83
3(6) 0.041	1.579e-002 CaSO4	9.212e-003 1.012e-002 -2.036 -1.99
-0.136	Fe_di(HS)3-	0.000e+000 0.000e+000 -411.744 -411.88
-0.635).041	Fe_di(HS)2	0.000e+000 0.000e+000 -274.530 -274.48
-0.187	S-2	0.000e+000 0.000e+000 -146.277 -146.91
0.041	HS-	0.000e+000 0.000e+000 -139.241 -139.42
0.041 5(-2)	0.000e+000 H2S	0.000e+000 0.000e+000 -137.962 -137.92
0.041 O(0)	3.828e-004 02	1.914e-004 2.102e-004 -3.718 -3.67
0.044	NaOH	4.783e-013 5.253e-013 -12.320 -12.28
-0.136	NaCO3-	1.378e-009 1.007e-009 -8.861 -8.99

	_	TOLAL U	= 3.38//246	3+00T	
		distribution o	ispecies		
T				Log	Log
Log Gamma	Species	Molality	Activity	Molality	Activity
Gallila	H+	4.770e-006	3.681e-006	-5.321	-5.434
-0.113	OH-	4.151e-009	2.696e-009	-8.382	-8.569
-0.187	H2O	5.551e+001	9.911e-001	1.744	-0.004
0.000		5.551e+001	9.911e-001	1./44	-0.004
C(-4) 0.041	0.000e+000 CH4	0.000e+000	0.000e+000	-141.384	-141.344
C(4)	1.389e-001 CC2	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	CaH003+	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
0.041	003-2	7.456e-007	1.831e-007	-6.128	-6.737
-0.610	MnH003+	1.037e-007	7.579e-008	-6.984	-7.120
-0.136	Fe_diCO3	9.031e-008	9.917e-008	-7.044	-7.004
0.041	MajCO3	3.995e-008	4.388e-008	-7.398	-7.358
0.041	Nacco3-	1.376e-009	1.006e-009	-8.861	-8.997
-0.136	MnCO3	7.837e-010	8.606e-010	-9.106	-9.065
0.041 Ca	1.476e-001			0.000	
-0.568	Ca+2	1.293e-001	3.498e-002 1.012e-002	-0.889	-1.456
0.041	CaSO4	9.213e-003		-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	CaH904+	2.985e-007	2.182e-007	-6.525	-6.661
-0.136	CaOH+	2.139e-009	1.563e-009	-8.670	-8.806
Cl -0.181	2.367e-001 Cl-	2.367e-001	1.559e-001	-0.626	-0.807
-0.136	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
0.041	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_dis04	5.300e-006	5.820e-006	-5.276	-5.235
0.041	Fe_dico3	9.031e-008	9.917e-008	-7.044	-7.004
0.041	Fe_diOH+	2.631e-009	1.923e-009	-8.580	-8.716
-0.136	Fe_diHSO4+	1.927e-010	1.408e-010	-9.715	-9.851
-0.136	Fe_di(HS)2	0.000e+000	0.000e+000	-274.593	-274.553
0.041	Fe_di.(HS)3-	0.000e+000	0.000e+000	-411.808	-411.944
-0.136 Fe_tri	2.542e-005				
-0.136	Fe_tri(OH)2+	2.416e-005	1.766e-005	-4.617 6.150	-4.753 -6.703
-0.545	Fe_triOH+2 Fe_tri(OH)3	6.941e-007 5.577e-007	1.980e-007 6.125e-007	-6.159	-6.703 -6.213
0.041	re_tri (OH) 3 Fe tri SO4+		1.810e-009	-6.254 9.606	
-0.136	_	2.477e-009		-8.606 o 710	-8.742
-1.226	Fe_tri+3	1.915e-009	1.139e-010	-8.718	-9.944

	Fe_triCl+2	1 879-009	5.362e-010	-8.726	-9.271	CO2(g) 0.55 -0.92 -1.47 CO2
-0.545	Fe_triCl2+		3.733e-010	-9.292	-9.428	Dolomite -1.44 -18.53 -17.09 Cavg(CO3)2 Gypsum 0.28 -4.30 -4.58 CaSO4:2H2O
-0.136	Fe_tri (OH) 4-		1.504e-010	-9.687	-9.823	H2(g) -41.21 -44.36 -3.15 H2 H20(g) -1.51 -0.00 1.51 H20
-0.136						H2S(g) -136.92 -137.92 -1.00 H2S
-2.179	Fe_tri2(OH)2+4		1.055e-012	-9.798	-11.977	Halite -5.92 -4.34 1.58 NaCl Hausmannite -8.92 52.11 61.03 Mn3O4
-0.136	Fe_tri(SO4)2-		5.740e-011	-10.105	-10.241	Manganite -1.10 24.24 25.34 MnOOH O2(g) -0.79 -3.68 -2.89 O2
-3.405	Fe_tri3(OH)4+5		3.893e-015	-11.005	-14.410	Pyrochroite -11.57 3.63 15.20 Mn(CH)2 Pyrolusite 3.46 44.84 41.38 MnC2
0.041	Fe_triCl3	5.300e-012	5.820e-012	-11.276	-11.235	Rhodochrosite
-0.545	Fe_triH9O4+2	6.254e-014	1.784e-014	-13.204	-13.749	Reaction step 4.
H(0)	0.000e+000 H2	0.000e+000	0.000e+000	-44.396	-44.355	Using solution 1.
0.041 K	5.270e-005					Using pure phase assemblage 1. Using kinetics 1. Kinetics defined in simulation 2.
-0.181	K+	5.222e-005	3.440e-005	-4.282	-4.464	Kinetics 1. Kinetics defined in simulation 2.
-0.136	KSO4-	4.793e-007	3.503e-007	-6.319	-6.456	
	KOH	2.924e-014	3.211e-014	-13.534	-13.493	Time step: 10800 seconds (Incremented time: 14400 sec
0.041 Mg	9.719e-004	0.054 004	0.544 004	2 000	2 500	Rate name Delta Moles Total Moles Reactant Coefficient
-0.523	Mg+2		2.511e-004	-3.078	-3.600	Fe_di_ax -5.450e-005 9.999e-001 Fe_di
0.041	MgS04	7.770e-005	8.533e-005	-4.110	-4.069	-1 F <u>e</u> tri
-0.136	MgHCO3+	5.778e-005	4.223e-005	-4.238	-4.374	1
0.041	MgCO3	3.995e-008	4.388e-008	-7.398	-7.358	Phase assemblage
-0.136	MgCH+	3.359e-010	2.455e-010	-9.474	-9.610	Moles in assemb
-0.136 Mn(2)	3.951e-007 Mn+2	2 2280 007	5.917e-008	-6.652	-7.228	Phase SI log IAP log KT Initial Delta
-0.576				-6.984		
-0.136	MnHCO3+		7.579e-008		-7.120 7.42F	02(g) -0.79 -3.68 -2.89 1.000e+001 1.00 1.363e-005
-0.136	MnCl+		3.758e-008	-7.289	-7.425	Solution composition
0.041	MnSO4		1.525e-008	-7.857	-7.817	
0.041	MnCl2		2.557e-009	-8.633	-8.592	Elements Molality Moles
0.041	MnCO3	7.837e-010	8.606e-010	-9.106	-9.065	C 1.389e-001 1.389e-001 Ca 1.476e-001 1.476e-001
-0.136	MnCl3-	1.502e-010	1.098e-010	-9.823	-9.959	Cl 2.367e-001 2.367e-001 Fe_di 8.109e-005 8.109e-005
-0.136	MnCH+	5.604e-013	4.096e-013	-12.251	-12.388	Fe tri 7.991e-005 7.991e-005 K 5.270e-005 5.270e-005
n(3)	4.532e-017	4 E225 017	2.696e-018	-16.344	-17.569	Mg 9.719e-004 9.719e-004
1.226	Mn+3	4.332E-017	2.0900-010	-10.344	-17.309	Mn 3.951e-007 3.951e-007 Na 4.183e-004 4.183e-004
Va	4.183e-004 Na+	4.132e-004	2.950e-004	-3.384	-3.530	S 1.579e-002 1.579e-002
-0.146	NaSO4-	2.933e-006	2.143e-006	-5.533	-5.669	
-0.136	NaHCO3	2.171e-006	2.384e-006	-5.663	-5.623	pH = 5.433 Charge bal
0.041	NaCO3-	1.376e-009	1.006e-009	-8.861	-8.997	pe = 15.169 Adjusted t equilibrium
-0.136	NaOH	4.780e-013	5.249e-013	-12.321	-12.280	Activity of water = 0.991 Ionic strength = 4.067e-001
).041)(0)	3.828e-004					Mass of water (kg) = 1.000e+000 Total alkalinity (eg/kg) = 2.975e-002
0.041	O2	1.914e-004	2.102e-004	-3.718	-3.677	Total CC2 (mol/kg) = 1.389e-001 Temperature (deg C) = 25.000
5(-2)	0.000e+000 H2S	0.000-1000	0.000e+000	127 061	127 001	Electrical balance (eg) = 2.542e-014 Percent error, 100*(Cat- 2n)/(Cat+ 2n) = 0.00 Tterations = 34
.041						
0.187	HS-		0.000e+000			Total H = 1.110421e+002 Total O = 5.587726e+001
0.635	S-2		0.000e+000			Distribution of species
0.041	Fe_di(HS)2		0.000e+000			
-0.136	Fe_di(HS)3-	0.000e+000	0.000e+000	-411.808	-411.944	Log L
5(6)	1.579e-002 CaSO4	9.213e_nn3	1.012e-002	-2.036	-1.995	Species Molality Activity Molality Act Camma
0.041	504-2		1.449e-003	-2.188	-2.839	
-0.651						-0.113
0.041	Mg904		8.533e-005	-4.110	-4.069	-0.187 CH- 4.143e-009 2.691e-009 -8.383 -
	Fe_di <i>S</i> 04	5.300e-006	5.820e-006	-5.276	-5.235	H2O 5.551e+001 9.911e-001 1.744 -
		0.005 -:	0 445		-5.669	C(-4) 0.000e+000 CH4 0.000e+000 0.000e+000 -141.384 -14
0.041	NaSO4-		2.143e-006	-5.533		0.041 C(4) 1.389e-001
0.041 -0.136			2.143e-006 5.187e-007	-5.533 -6.149	-6.285	
0.041 -0.136 -0.136	NaSO4-	7.097e-007				0.041 CO2 1.093e-001 1.200e-001 -0.961 -
0.041 -0.136 -0.136 -0.136	NaSO4- HSO4-	7.097e-007 4.793e-007	5.187e-007	-6.149	-6.285	0.041 HCO3- 2.039e-002 1.435e-002 -1.691 -
0.041 -0.136 -0.136 -0.136 -0.136	NaSO4- HSO4- KSO4-	7.097e-007 4.793e-007 2.985e-007	5.187e-007 3.503e-007	-6.149 -6.319	-6.285 -6.456	0.041 +003- 2.039e-002 1.435e-002 -1.691 - -0.152 CaH003+ 9.101e-003 6.407e-003 -2.041 -
0.041 0.136 0.136 0.136 0.136 0.136 0.041	NaSO4- HSO4- KSO4- CaHSO4+	7.097e-007 4.793e-007 2.985e-007 1.389e-008	5.187e-007 3.503e-007 2.182e-007	-6.149 -6.319 -6.525	-6.285 -6.456 -6.661	0.041 -0.152 -0.152 -0.152 -0.152 MgHCO3+ 2.039e-002 1.435e-002 -1.691 - 9.101e-003 6.407e-003 -2.041 - MgHCO3+ 5.771e-005 4.218e-005 -4.239 -
0.041 0.136 0.136 0.136 0.136 0.136 0.041 0.136	NaSO4- HSO4- KSO4- CaHSO4+ MnSO4	7.097e-007 4.793e-007 2.985e-007 1.389e-008 2.477e-009	5.187e-007 3.503e-007 2.182e-007 1.525e-008	-6.149 -6.319 -6.525 -7.857	-6.285 -6.456 -6.661 -7.817	0.041 -0.152 -0.152 -0.152 -0.152 -0.152 -0.152 -0.152 -0.154 -0.155 -0.156 -0.156 -0.157 -0.157 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136
0.041 -0.136 -0.136 -0.136 -0.136 0.041 -0.136 -0.136	Naso4- HSO4- KSO4- CaHSO4+ MnsO4 Fe_trisO4+	7.097e-007 4.793e-007 2.985e-007 1.389e-008 2.477e-009 1.927e-010	5.187e-007 3.503e-007 2.182e-007 1.525e-008 1.810e-009	-6.149 -6.319 -6.525 -7.857 -8.606	-6.285 -6.456 -6.661 -7.817 -8.742	0.041 -0.152 -0.152 -0.152 -0.152 -0.152 -0.136 Fe_diHCO3+ -0.136
0.041 -0.136 -0.136 -0.136 -0.136 0.041 -0.136 -0.136	NaSO4- HSO4- KSO4- CaHSO4+ MrSO4 Fe_triSO4+ Fe_diHSO4+	7.097e-007 4.793e-007 2.985e-007 1.389e-008 2.477e-009 1.927e-010 7.854e-011	5.187e-007 3.503e-007 2.182e-007 1.525e-008 1.810e-009 1.408e-010	-6.149 -6.319 -6.525 -7.857 -8.606 -9.715	-6.285 -6.456 -6.661 -7.817 -8.742 -9.851	0.041 -0.152 -0.152 -0.152 -0.152 -0.136 -0.136 -0.136 -0.136
0.041 0.136 0.136 0.136 0.136 0.041 0.136 0.136 0.136	NaSO4- HSO4- KSO4- CaHSO4+ MrSO4 Fe_triSO4+ Fe_tri(SO4)2-	7.097e-007 4.793e-007 2.985e-007 1.389e-008 2.477e-009 1.927e-010 7.854e-011	5.187e-007 3.503e-007 2.182e-007 1.525e-008 1.810e-009 1.408e-010 5.740e-011	-6.149 -6.319 -6.525 -7.857 -8.606 -9.715 -10.105	-6.285 -6.456 -6.661 -7.817 -8.742 -9.851 -10.241	0.041 -0.152 -0.152 -0.152 -0.152 -0.152 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.041 -0.041 -0.041 -0.041 -0.041 -0.041 -0.041 -0.041 -0.041 -0.041 -0.052 -0.0539-002 -0.1369-006 -0.1369-006 -0.079-006 -
0.041 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136	NaSO4- HSO4- KSO4- CaHSO4+ MrSO4 Fe_triSO4+ Fe_tri(SO4)2-	7.097e-007 4.793e-007 2.985e-007 1.389e-008 2.477e-009 1.927e-010 7.854e-011	5.187e-007 3.503e-007 2.182e-007 1.525e-008 1.810e-009 1.408e-010 5.740e-011	-6.149 -6.319 -6.525 -7.857 -8.606 -9.715 -10.105	-6.285 -6.456 -6.661 -7.817 -8.742 -9.851 -10.241	0.041 -0.152 -0.152 -0.152 -0.152 -0.152 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.041 -0.041 -0.041 -0.041 -0.061
0.041 -0.136 -0.136 -0.136 -0.136 0.041 -0.136 -0.136 -0.136	NaSO4- HSO4- KSO4- CaHSO4+ MrSO4 Fe_triSO4+ Fe_tri(SO4)2- Fe_triHSO4+2	7.097e-007 4.793e-007 2.985e-007 1.389e-008 2.477e-009 1.927e-010 7.854e-011 6.254e-014	5.187e-007 3.503e-007 2.182e-007 1.525e-008 1.810e-009 1.408e-010 5.740e-011 1.784e-014	-6.149 -6.319 -6.525 -7.857 -8.606 -9.715 -10.105	-6.285 -6.456 -6.661 -7.817 -8.742 -9.851 -10.241	0.041 -0.152 -0.152 -0.152 -0.152 -0.152 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.041 -0.041 -0.041 -0.041 -0.041 -0.041 -0.053 -0.041 -0.0610 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.041 -0
0.041 -0.136 -0.136 -0.136 -0.136	NaSO4- HSO4- KSO4- CaHSO4+ MrSO4 Fe_trisO4+ Fe_tri(SO4)2- Fe_triHSO4+2	7.097e-007 4.793e-007 2.985e-007 1.389e-008 2.477e-009 1.927e-010 7.854e-011 6.254e-014 SI log 1	5.187e-007 3.503e-007 2.182e-007 1.525e-008 1.810e-009 1.408e-010 5.740e-011 1.784e-014 indices	-6.149 -6.319 -6.525 -7.857 -8.606 -9.715 -10.105 -13.204	-6.285 -6.456 -6.661 -7.817 -8.742 -9.851 -10.241	0.041 -0.152 -0.152 -0.152 -0.152 -0.152 -0.153 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.041 -0.
0.041 -0.136 -0.136 -0.136 -0.136 0.041 -0.136 -0.136 -0.136	NaSO4- HSO4- KSO4- CaHSO4+ MrSO4 Fe_triSO4+ Fe_tri(SO4)2- Fe_triHSO4+2	7.097e-007 4.793e-007 2.985e-007 1.389e-008 2.477e-009 1.927e-010 7.854e-011 6.254e-014	5.187e-007 3.503e-007 2.182e-007 1.525e-008 1.810e-009 1.409e-010 5.740e-011 1.784e-014 indices EAP log KT 29 -4.36 19 -8.34	-6.149 -6.319 -6.525 -7.857 -8.606 -9.715 -10.105 -13.204 Caso4 Caco3	-6.285 -6.456 -6.661 -7.817 -8.742 -9.851 -10.241	0.041 -0.152 -0.152 -0.152 -0.152 -0.152 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.136 -0.041 -0.041 -0.041 -0.041 -0.041 -0.041 -0.051 -0.0610 -0.136 -0.136 -0.136 -0.136 -0.136 -0.081 -0.085 -0

0.041	MnCO3	7.816e-010	8.584e-010	-9.107	-9.066	Na.	4.183e-004 Na+	4.132e-004 2.951e-004 -3.384 -3.530
Ca	1.476e-001 Ca+2	1.293e-001	3.499e-002	-0.888	-1.456	-0.146	NaSO4-	2.933e-006 2.144e-006 -5.533 -5.669
-0.568	CaSO4	9.215e-003	1.012e-002	-2.036	-1.995	-0.136	NaHCO3	2.168e-006 2.381e-006 -5.664 -5.623
0.041	CaHCO3+		6.407e-003	-2.041	-2.193	0.041	NaCO3-	1.372e-009 1.003e-009 -8.863 -8.999
-0.152	CaCO3		1.073e-005	-5.010	-4.969	-0.136	NaCH	4.772e-013 5.240e-013 -12.321 -12.281
0.041						0.041		4.7726-013 3.2406-013 -12.321 -12.201
-0.136	CaH904+		2.186e-007	-6.524	-6.660	0(0)	3.828e-004 02	1.914e-004 2.102e-004 -3.718 -3.677
-0.136	CaOH+	2.136e-009	1.561e-009	-8.670	-8.807	0.041 S(-2)	0.000e+000	
Cl	2.367e-001 Cl-	2.367e-001	1.559e-001	-0.626	-0.807	0.041	H2S	0.000e+000 0.000e+000 -137.960 -137.919
-0.181	Fe_diCl+	3.978e-006	2.907e-006	-5.400	-5.537	-0.187	HS-	0.000e+000 0.000e+000 -139.240 -139.427
-0.136	MnCl+		3.759e-008	-7.289	-7.425	-0.635	S-2	0.000e+000 0.000e+000 -146.277 -146.912
-0.136	Fe_triCl+2		1.692e-009	-8.227	-8.772	0.041	Fe_di(HS)2	0.000e+000 0.000e+000 -274.815 -274.774
-0.545	MnCl2				-8.592	-0.136	Fe_di(HS)3-	0.000e+000 0.000e+000 -412.028 -412.164
0.041			2.558e-009	-8.633		S(6)	1.579e-002	0.015 000 1.010 000 0.005 1.005
-0.136	Fe_triCl2+		1.178e-009	-8.793	-8.929	0.041	Ca.904	9.215e-003 1.012e-002 -2.036 -1.995
-0.136	MnCl3-		1.098e-010	-9.823	-9.959	-0.651	SO4-2	6.490e-003 1.450e-003 -2.188 -2.839
0.041	Fe_triCl3	1.672e-011	1.836e-011	-10.777	-10.736	0.041	MgSO4	7.772e-005 8.535e-005 -4.109 -4.069
Fe <u>d</u> i	8.109e-005 Fe_di+2	4.735e-005	1.351e-005	-4.325	-4.869	0.041	Fe <u>di</u> 304	3.171e-006 3.482e-006 -5.499 -5.458
-0.545	Fe_diH003+	2.653e-005	1.939e-005	-4.576	-4.712	-0.136	NaSO4-	2.933e-006 2.144e-006 -5.533 -5.669
-0.136	Fe_diCl+		2.907e-006	-5.400	-5.537	-0.136	H904-	7.110e-007 5.196e-007 -6.148 -6.284
-0.136	Fe_dis04		3.482e-006	-5.499	-5.458	-0.136	KSO4-	4.794e-007 3.503e-007 -6.319 -6.456
0.041							CaHSO4+	2.991e-007 2.186e-007 -6.524 -6.660
0.041	Fe_di003		5.916e-008	-7.269	-7.228	-0.136	Mn904	1.390e-008 1.526e-008 -7.857 -7.816
-0.136	Fe_diOH+		1.148e-009	-8.804	-8.940	0.041	Fe_triSO4+	7.814e-009 5.711e-009 -8.107 -8.243
-0.136	Fe_diHSO4+		8.440e-011	-9.937	-10.074	-0.136	Fe_tri(\$04)2-	2.478e-010 1.811e-010 -9.606 -9.742
0.041	Fe_di(HS)2	0.000e+000	0.000e+000	-274.815	-274.774	-0.136	Fe diH904+	1.155e-010 8.440e-011 -9.937 -10.074
-0.136	Fe_di(HS)3-	0.000e+000	0.000e+000	-412.028	-412.164	-0.136	Fe_triHSO4+2	1.976e-013 5.639e-014 -12.704 -13.249
Fe_tri	7.991e-005 Fe_tri(OH)2+	7 5950_005	5.551e-005	-4.119	-4.256	-0.545		
-0.136			6.236e-007	-5.660	-6.205			Saturation indices
-0.545	Fe_triOH+2						M	OT 1 TAD 1 MT
0.041	Fe_tri(OH)3		1.922e-006	-5.757	-5.716		Phase	SI log IAP log KT
-0.136	Fe_triSO4+		5.711e-009	-8.107	-8.243		Anhydrite Aragonite	0.07 -4.29 -4.36 CaSO4 0.14 -8.19 -8.34 CaCO3
-1.226	Fe_tri+3		3.593e-010	-8.219	-9.445		Calcite CH4(g)	0.29 -8.19 -8.48 CaCC3 -138.48 -141.34 -2.86 CH4
-0.545	Fe_triCl+2	5.929e-009	1.692e-009	-8.227	-8.772		CO2(g) Dolomite	0.55 -0.92 -1.47 CC2 -1.44 -18.53 -17.09 CaMg(CC3)2
-0.136	Fe_triCl2+	1.612e-009	1.178e-009	-8.793	-8.929		Gypsum H2(g)	0.28 -4.30 -4.58 CaSO4:2H2O -41.21 -44.36 -3.15 H2
-2.179	Fe_tri2(OH)2+4	1.580e-009	1.047e-011	-8.801	-10.980		H2O(g) H2S(g)	-1.51 -0.00 1.51 H20 -136.92 -137.92 -1.00 H2S
-0.136	Fe_tri(OH)4-	6.448e-010	4.713e-010	-9.191	-9.327		Halite Hausmannite	-5.92 -4.34 1.58 NaCl -8.92 52.11 61.03 Mn3O4
-3.405	Fe_tri3(OH)4+5	3.081e-010	1.214e-013	-9.511	-12.916		Manganite 02(g)	-1.11 24.23 25.34 MnOOH -0.79 -3.68 -2.89 C2
-0.136	Fe_tri(SO4)2-	2.478e-010	1.811e-010	-9.606	-9.742		Pyrochroite	-11.57 3.63 15.20 Mn(CH)2 3.46 44.84 41.38 MnC2
	Fe_triCl3	1.672e-011	1.836e-011	-10.777	-10.736		Pyrolusite Rhodochrosite	-2.84 -13.97 -11.13 MnCC3
0.041	Fe_triH904+2	1.976e-013	5.639e-014	-12.704	-13.249		Sulfur	-101.60 -96.71 4.88 S
-0.545 H(0)	0.000e+000					Reaction ste	_	
0.041	H2	0.000e+000	0.000e+000	-44.396	-44.355	Using soluti Using pure p	on 1. hase assemblage	1.
K	5.270e-005 K+	5.222e-005	3.440e-005	-4.282	-4.463	Using kineti		Kinetics defined in simulation 2.
-0.181	KS04-	4.794e-007	3.503e-007	-6.319	-6.456	Kinetics 1.	Kinetics defin	ed in simulation 2.
-0.136	KOH	2.919e-014	3.206e-014	-13.535	-13.494		Time step: 216	00 seconds (Incremented time: 36000 seconds)
0.041 Mg	9.719e-004					Opefficient	Rate name	Delta Moles Total Moles Reactant
-0.523	Mg+2	8.364e-004	2.511e-004	-3.078	-3.600		Fe_di_ax	-5.198e-005 9.999e-001 Fe_di
0.041	MgSO4	7.772e-005	8.535e-005	-4.109	-4.069	-1	10_01_01	Fe_tri
-0.136	MgHCO3+	5.771e-005	4.218e-005	-4.239	-4.375	1		10_41
	MgCO3	3.984e-008	4.375e-008	-7.400	-7.359			Phase assemblage
0.041	MgCH+	3.354e-010	2.451e-010	-9.474	-9.611			*1
-0.136 Mn(2)	2 054 005		F 010 057	-6.652	7 000	D 21	Phase	Moles in assemblage SI log IAP log KT Initial Final
	3.951e-007	0.000 000			-7.228	Delta		
-0.576	Mn+2	2.229e-007			D 404	1		0.00
	Mn+2 MnHCO3+	1.036e-007	7.572e-008	-6.985	-7.121	1.300e-005	02 (g)	-0.78 -3.68 -2.89 1.000e+001 1.000e+001-
-0.576	Mn+2	1.036e-007			-7.121 -7.425	1.300e-005	02 (g)	-0.78 -3.68 -2.89 1.000e+001 1.000e+001-
-0.576 -0.136 -0.136	Mn+2 MnHCO3+	1.036e-007 5.144e-008	7.572e-008	-6.985		1.300e-005 	02 (g)	
-0.576 -0.136 -0.136 0.041	Mn+2 MnHCO3+ MnCl+	1.036e-007 5.144e-008 1.390e-008	7.572e-008 3.759e-008	-6.985 -7.289	-7.425	1.300e-005 	O2(g) Elements	
-0.576 -0.136 -0.136 0.041 0.041	Mn+2 Mn+1003+ MnCl+ MnS04	1.036e-007 5.144e-008 1.390e-008 2.329e-009	7.572e-008 3.759e-008 1.526e-008	-6.985 -7.289 -7.857	-7.425 -7.816	1.300e-005 	Elements C	-Solution composition
-0.576 -0.136 -0.136 0.041 0.041	Mn+2 Mn+COS+ MnCl+ MnSO4 MnCl2	1.036e-007 5.144e-008 1.390e-008 2.329e-009 7.816e-010	7.572e-008 3.759e-008 1.526e-008 2.558e-009	-6.985 -7.289 -7.857 -8.633	-7.425 -7.816 -8.592	1.300e-005	Elements C Ca Cl	-Solution composition
-0.576 -0.136 -0.136 0.041 0.041 -0.136	Mn+2 MnHC03+ MnC1+ MnS04 MnC12 MnC03	1.036e-007 5.144e-008 1.390e-008 2.329e-009 7.816e-010 1.503e-010	7.572e-008 3.759e-008 1.526e-008 2.558e-009 8.584e-010	-6.985 -7.289 -7.857 -8.633 -9.107	-7.425 -7.816 -8.592 -9.066	1.300e-005 	Elements C Ca Cl Fe_di Fe_tri	Molality Moles 1.389e-001 1.389e-001 1.476e-001 1.476e-001 2.367e-001 2.367e-001 2.911e-005 2.911e-005 1.319e-004 1.319e-004
-0.576 -0.136 -0.136 0.041 0.041	Mn+2 Mn+003+ MnC1+ Mn504 MnC12 Mn003 MnC13- MnOH+ 4.541e-017	1.036e-007 5.144e-008 1.390e-008 2.329e-009 7.816e-010 1.503e-010 5.596e-013	7.572e-008 3.759e-008 1.526e-008 2.558e-009 8.584e-010 1.098e-010 4.090e-013	-6.985 -7.289 -7.857 -8.633 -9.107 -9.823 -12.252	-7.425 -7.816 -8.592 -9.066 -9.959 -12.388	1,300e-005 ———————————————————————————————————	Elements C Ca Cl Fe_dii Fe_tri K	-Solution composition
-0.576 -0.136 -0.136 0.041 0.041 0.041 -0.136	Mn+2 Mn+CO3+ MnCl+ MnCO3 MnCO3 MnCO3- MnCH+	1.036e-007 5.144e-008 1.390e-008 2.329e-009 7.816e-010 1.503e-010 5.596e-013	7.572e-008 3.759e-008 1.526e-008 2.558e-009 8.584e-010 1.098e-010	-6.985 -7.289 -7.857 -8.633 -9.107 -9.823 -12.252	-7.425 -7.816 -8.592 -9.066 -9.959	1,300e-005	Elements C Ca Cl Fe_di Fe_tri K	-Solution composition

	S	1.579e-002	1.579e-002			1	Fe_tri(CH)3	2.884e-006	3.167e-006	-5.540	-5.499
		Description of	f solution			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
			= 5.433 = 15.170		e balance ted to redox	-1.226	Fe_triCl+2	9.818e-009	2.801e-009	-8.008	-8.553
equilibriu	Acti	vity of water	= 0.991			-0.545	Fe_tri2(OH)2+4	4.318e-009	2.860e-011	-8.365	-10.544
	I	ionic strength of water (kg)	= 4.067e-0			-2.179	Fe_triCl2+	2.669e-009	1.950e-009	-8.574	-8.710
	Total alkal	inity (eg/kg) . CO2 (mol/kg)	= 2.980e-(= 1.389e-(002		-0.136	Fe_tri3(OH)4+5		5.474e-013	-8.857	-12.262
	Temper	ature (deg C) balance (eg)	= 25.000 = 2.537e-0			-3.405	Fe_tri(OH)4-		7.752e-010	-8.974	-9.111
Percent e	rror, 100* (Cat- An)/(Cat+ An) Iterations	= 0.00			-0.136	Fe_tri(SO4)2-		3.000e-010	-9.387	-9.523
		Total H	= 1.110421e = 5.587729e			-0.136	Fe_triCl3		3.041e-011	-10.558	-10.517
		Distribution o		STOOL		0.041	Fe_triH904+2		9.353e-014	-12.484	-13.029
		DISCI DUCIOI (or sherres			-0.545 H(0)	0.000e+000	3.2700-013	J.555E-014	-12.404	-13.029
Tow				Log	Log	0.041	H2	0.000e+000	0.000e+000	-44.396	-44.355
Log	Species	Molality	Activity	Molality	Activity	K	5.270e-005	E 2220 00E	2 440- 005	4 202	1 163
Gamma		4 705 005	2 602 006	E 200	E 400	-0.181	K+		3.440e-005	-4.282	-4.463
-0.113	H+		3.693e-006	-5.320	-5.433	-0.136	KSO4-		3.504e-007	-6.319	-6.455
-0.187	OH-		2.687e-009	-8.383	-8.571	0.041	KOH	2.915e-014	3.201e-014	-13.535	-13.495
0.000	H2O	5.551e+001	9.911e-001	1.744	-0.004	Mg	9.719e-004 Mg+2	8.365e-004	2.512e-004	-3.078	-3.600
C(-4)	0.000e+000 CH4	0.000e+000	0.000e+000	-141.384	-141.343	-0.522	MgSO4	7.773e-005	8.536e-005	-4.109	-4.069
0.041 C(4)	1.389e-001					0.041	MgHCO3+	5.765e-005	4.213e-005	-4.239	-4.375
0.041	CO2	1.094e-001	1.201e-001	-0.961	-0.920	-0.136	MgC03	3.973e-008	4.363e-008	-7.401	-7.360
-0.152	H003-	2.036e-002	1.434e-002	-1.691	-1.844	0.041	MgCH+	3.349e-010	2.447e-010	-9.475	-9.611
-0.152	CaHCO3+	9.090e-003	6.399e-003	-2.041	-2.194	-0.136 Mn(2)	3.951e-007				
-0.136	MgHCO3+	5.765e-005	4.213e-005	-4.239	-4.375	-0.576	Mn+2	2.230e-007	5.921e-008	-6.652	-7.228
0.041	CaCO3	9.743e-006	1.070e-005	-5.011	-4.971	-0.136	MnHCO3+	1.035e-007	7.565e-008	-6.985	-7.121
-0.136	Fe_diH003+	9.515e-006	6.954e-006	-5.022	-5.158	-0.136	MnCl+	5.146e-008	3.761e-008	-7.289	-7.425
0.041	NaHCO3	2.166e-006	2.379e-006	-5.664	-5.624	0.041	MnSO4	1.390e-008	1.527e-008	-7.857	-7.816
-0.610	003-2	7.412e-007	1.820e-007	-6.130	-6.740	0.041	MnCl2	2.330e-009	2.559e-009	-8.633	-8.592
-0.136	MnH003+	1.035e-007	7.565e-008	-6.985	-7.121	0.041	MnCO3	7.797e-010	8.562e-010	-9.108	-9.067
0.041	MgCO3	3.973e-008	4.363e-008	-7.401	-7.360	-0.136	MnCl3-	1.504e-010	1.099e-010	-9.823	-9.959
	Fe_diCO3	1.929e-008	2.118e-008	-7.715	-7.674		MnOH+	5.589e-013	4.085e-013	-12.253	-12.389
0.041	NaCO3-	1.369e-009	1.000e-009	-8.864	-9.000	-0.136 Mn(3)	4.550e-017	4 550 018	0.707.010	16 240	15.500
-0.136	MnCO3	7.797e-010	8.562e-010	-9.108	-9.067	-1.226	Mn+3	4.550 0 -017	2.707e-018	-16.342	-17.568
0.041 Ca	1.476e-001	4 000 004	2 400 000		4 455	Na.	4.183e-004 Na+	4.132e-004	2.951e-004	-3.384	-3.530
-0.568	Ca+2		3.499e-002	-0.888	-1.456	-0.146	NaSO4-	2.933e-006	2.144e-006	-5.533	-5.669
0.041	Ca904		1.012e-002	-2.035	-1.995	-0.136	NaHCO3	2.166e-006	2.379e-006	-5.664	-5.624
-0.152	CaHCO3+		6.399e-003	-2.041	-2.194	0.041	NaCO3-	1.369e-009	1.000e-009	-8.864	-9.000
0.041	CaCO3		1.070e-005	-5.011	-4.971	-0.136	NaOH	4.764e-013	5.232e-013	-12.322	-12.281
-0.136	CaHSO4+		2.190e-007	-6.523	-6.660	0.041 O(0)	3.828e-004				
-0.136	CaOH+	2.132e-009	1.558e-009	-8.671	-8.807	0.041	02	1.914e-004	2.102e-004	-3.718	-3.677
Cl	2.367e-001 Cl-	2.367e-001	1.559e-001	-0.626	-0.807	S(-2)	0.000e+000 H2S	0.000e+000	0.000e+000	-137.958	-137.918
-0.181	Fe_diCl+	1.428e-006	1.044e-006	-5.845	-5.981	0.041	HS-	0.000e+000	0.000e+000	-139.239	-139.427
-0.136	MnCl+	5.146e-008	3.761e-008	-7.289	-7.425	-0.187	S-2	0.000e+000	0.000e+000	-146.277	-146.912
-0.136	Fe_triCl+2	9.818e-009	2.801e-009	-8.008	-8.553	-0.635	Fe_di(HS)2	0.000e+000	0.000e+000	-275.258	-275.217
-0.545	Fe triCl2+	2.669e-009	1.950e-009	-8.574	-8.710	0.041	Fe_di(HS)3-	0.000e+000	0.000e+000	-412.471	-412.607
-0.136	MnCl2	2.330e-009	2.559e-009	-8.633	-8.592	-0.136 S(6)	1.579e-002				
0.041	MhCl3-		1.099e-010	-9.823	-9.959	0.041	CaSO4	9.216e-003	1.012e-002	-2.035	-1.995
-0.136	Fe triCl3		3.041e-011	-10.558	-10.517	-0.651	SO4-2	6.490e-003	1.450e-003	-2.188	-2.839
0.041 Fe_di	2.911e-005					0.041	MgSO4	7.773e-005	8.536e-005	-4.109	-4.069
-0.545	Fe_di+2	1.700e-005	4.851e-006	-4.769	-5.314	-0.136	NaSO4-	2.933e-006	2.144e-006	-5.533	-5.669
-0.136	Fe_diH003+	9.515e-006	6.954e-006	-5.022	-5.158	0.041	Fe_dis04	1.139e-006	1.251e-006	-5.944	-5.903
-0.136	Fe_diCl+	1.428e-006	1.044e-006	-5.845	-5.981	-0.136	HSO4-	7.123e-007	5.206e-007	-6.147	-6.284
0.041	Fe_dis04	1.139e-006	1.251e-006	-5.944	-5.903	-0.136 -0.136	KSO4-	4.794e-007	3.504e-007	-6.319	-6.455
	Fe_diCO3	1.929e-008	2.118e-008	-7.715	-7.674		CaHSO4+	2.996e-007	2.190e-007	-6.523	-6.660
0.041	Fe_diOH+	5.633e-010	4.117e-010	-9.249	-9.385	-0.136	MnSO4	1.390e-008	1.527e-008	-7.857	-7.816
-0.136	Fe_diHSO4+	4.154e-011	3.036e-011	-10.382	-10.518	0.041	Fe_triSO4+	1.294e-008	9.457e-009	-7.888	-8.024
-0.136	Fe_di(HS)2	0.000e+000	0.000e+000	-275.258	-275.217	-0.136	Fe_tri(SO4)2-	4.104e-010	3.000e-010	-9.387	-9.523
0.041	Fe_di(HS)3-	0.000e+000	0.000e+000	-412.471	-412.607	-0.136	Fe_diH904+	4.154e-011	3.036e-011	-10.382	-10.518
-0.136 Fe_tri	1.319e-004	4.05-	0.460			-0.136	Fe_triH904+2	3.278e-013	9.353e-014	-12.484	-13.029
-0.136	Fe_tri(OH)2+	1.253e-004	9.161e-005	-3.902	-4.038	-0.545		a			

----Saturation indices----

-5.987

-0.545

Fe_triOH+2

3.614e-006 1.031e-006 -5.442

Part										
		Phase SI lo	g IAP log KT		0.041	NaHCO3	2.165e-006	2.377e-006	-5.665	-5.624
Section Sect						Fe_diHCO3+	8.762e-007	6.403e-007	-6.057	-6.194
Company 1.00		Calcite 0.28	-8.20 -8.48 CaCO3			CO3-2	7.401e-007	1.818e-007	-6.131	-6.740
Section Sect		CC(g) 0.55	-0.92 -1.47 002			MnHCC3+	1.035e-007	7.562e-008	-6.985	-7.121
		Gypsum 0.28	-4.30 -4.58 CaSO4:2H20			MgCO3	3.967e-008	4.357e-008	-7.401	-7.361
Section 1,000		H2O(a) -1.51	-0.00 1.51 H2O			Fe_diCO3	1.775e-009	1.949e-009	-8.751	-8.710
Negation 1.11 34.0 3.0		Halite -5.92	-4.34 1.58 NaCl			NaCO3-	1.367e-009	9.987e-010	-8.864	-9.001
		Manganite -1.11	24.23 25.34 MnOOH			MnCO3	7.787e-010	8.551e-010	-9.109	-9.068
Selection 18 18 18 18 18 18 18 1		Pyrochroite -11.57	3.63 15.20 Mn(OH)2							
Section Sect		Rhodochrosite -2.84 -	13.97 -11.13 Mhccc3		-0.568					
Part			96.71 4.88 S		0.041					
Marine M		_			-0.152					
Second S					0.041					
Part		Usually caused by KINETIC	S, REACTION, or diffuse 1	ayer	-0.136	CaH904+				
## Service convertentions in the difficult page. Call	calculation.		steps in early part of KI	NEITCS	-0.136	CaOH+	2.131e-009	1.557e-009	-8.672	-8.808
Chirp Prese present presen		r negative concentrations i			Cl	2.367e-001 Cl-	2.367e-001	1.559e-001	-0.626	-0.807
Number of defined in similarion 2	Using pure p	hase assemblage 1.	fined in simulation 2.		-0.181	Fe diCl+			-6.881	
The stop 5000 secunds (Incremented time 8600 secunds)	_									
A) seconds)	-0.136					
Conficiency Part Conficiency Conficie		-			-0.545					
The part Par	Coefficient	- Detta Pol		-	-0.136					
Page	_1	Fe_di_ox -2.642e-0	05 9.998e-001 Fe <u>d</u> i		0.041					
Section Color Co			Fe_tri		-0.136					
Pare	_	Dhaco ac	complace				J.J2JE-011	3.0300-011	-10.470	-10.457
Part		riase as	Selblage				1.567e-006	4.470e-007	-5.805	-6.350
Delta		ri (r. 1				Fe_diH003+	8.762e-007	6.403e-007	-6.057	-6.194
6.678-006	Delta	Hase SI 10	g IAP 10g KI: INICIAL	HIEL		Fe_diCl+	1.316e-007	9.618e-008	-6.881	-7.017
Solution composition	5 500 005	O2 (g) -0.78	-3.68 -2.89 1.000e+001	1.000e+001-		Fe_dis04	1.049e-007	1.152e-007	-6.979	-6.938
Elements Molality Molas	6.607/e-006					Fe_diCO3	1.775e-009	1.949e-009	-8.751	-8.710
Elements Molality Moles -0.156 Ps_diffES) 3.836-012 2.800-02 -11.47 -11.533 Ca 1.476-03 -1		Solutian c	amposition			Fe_diOH+	5.186e-011	3.790e-011	-10.285	-10.421
C		Elements Molali	ty Moles			Fe_diHSO4+	3.831e-012	2.800e-012	-11.417	-11.553
Cl. 2.367e-001 2.367e-001 2.367e-001 1.505e-001			01 1.389e-001			Fe_di(HS)2	0.000e+000	0.000e+000	-276.293	-276.252
Fe Fr 1.583e-004 1.583e		Cl 2.367e-0	01 2.367e-001			Fe_di(HS)3-	0.000e+000	0.000e+000	-413.505	-413.641
Re_init(H)						1.583e-004				
Na						Fe_tri(OH)2+	1.505e-004	1.100e-004	-3.823	
S		Na 4.183e-0	04 4.183e-004		-0.545	Fe_triOH+2	4.341e-006	1.238e-006	-5.362	-5.907
Part		S 1.579e-0	02 1.579e-002		0.041	Fe_tri(OH)3	3.459e-006	3.798e-006	-5.461	-5.420
Family F		Description	of solution		-0.136	Fe_tri504+	1.556e-008	1.137e-008	-7.808	-7.944
February			nH = 5.432 Charos	e balance		Fe_tri+3	1.203e-008	7.153e-010	-7.920	-9.146
Activity of water 0.991	equilibrium		pe = 15.170 Adjust			Fe_triCl+2	1.180e-008	3.368e-009	-7.928	-8.473
Mess of water (Fig) = 1.000e+000 7.00e+001 7.01al cult (mol/kg) = 2.988e-002 1.389e-001 7.01al cult (mol/kg) = 1.271e-013 7.00al cult (mol/kg) = 1.20al cult (mol/kg)		Activity of wat Tonic streng	er = 0.991 th = 4.066e-001			Fe_tri2(OH)2+4	6.232e-009	4.128e-011	-8.205	-10.384
Total Crg (mol/kg) = 1.389e-001 Reperature (eg) = 5.5000 Recreate error, 100*(Cat- An)/(Cat+ An) = 0.00 Percent error, 100*(Cat- An)/(Cat+ An) = 8.5000 Total O = 5.587730e+001 Log Species Molality Activity Molality Activity Remain H		Mass of water (k	g) = 1.000e+000			Fe_triCl2+	3.209e-009	2.345e-009	-8.494	-8.630
Ferroant error, 100* (Cat. Am) / (Cat. Am) = 1.721e-013 = 0.00 Tterations = 85 Ttotal H = 1.110421e+002 Total O = 5.587730e+001 -0.136 Fe_tri (GM)2-		Total CO2 (mol/k	g) = 1.389e-001			Fe_tri3(OH)4+5	2.407e-009	9.483e-013	-8.619	-12.023
Titerations = 85 Total O = 5.587730e+001	Parnant enn	Electrical balance (e	g) = 1.721e-013			Fe_tri(OH)4-	1.271e-009	9.289e-010	-8.896	-9.032
Total 0 = 5.587730e+001	racan en	Iteratio	ns = 85			Fe_tri(SO4)2-	4.935e-010	3.607e-010	-9.307	-9.443
Total Tota						Fe_triCl3	3.329e-011	3.656e-011	-10.478	-10.437
H(0) 0.000e+000 0.000e+000 0.000e+000 0.000e+000 0.44.396 -44.356 0.000e+000 0		Distributio	n of species			Fe_triHSO4+2	3.945e-013	1.125e-013	-12.404	-12.949
Commo			Ŧ	Torr			0 000	0.000~,000	M 20C	NA SEE
Red	Log	Operation 25.3.3.1	_	-			v.vuue+000	v.uue+000	-44.396	-44.355
-0.113	Camma	apecies Molali	cy ACCLIVICY MODALITY	MULTIVITY			5.222e-005	3.440e-005	-4.282	-4.463
0.187 H2O 5.551e+001 9.911e-001 1.744 -0.004 0.004 0.000e+000 0.000	0.113	H+ 4.790e-0	06 3.696e-006 -5.320	-5.432		K904-	4.794e-007	3.504e-007	-6.319	-6.455
H2O 5.551e+001 9.911e-001 1.744 -0.004 Mgr 9.719e-004 Mgr2 8.365e-004 2.512e-004 -3.078 -3.600		OH- 4.133e-0	09 2.684e-009 -8.384	-8.571		KOH	2.912e-014	3.198e-014	-13.536	-13.495
C(-4) 0.000e+000 CH4 0.000e+000 0.0000e+000 0.0000e+000 0.0000e+000 0.0000e+000 0.0000e+000 0.0000e+000 0.0000e+000 0.00000 0.0000e+000 0.0000e+000 0.0000e+000 0.0000e+000 0.0000e+000 0.0		H2O 5.551e+0	01 9.911e-001 1.744	-0.004			0.055	0.540		
0.041					-0.522	-				
-0.152			UU 0.000e+000 -141.384	-141.343	0.041	-				
0.041		1.389e-001 CO2 1.094e-0	01 1.201e-001 -0.961	-0.920	-0.136	-				
-0.152					0.041	-				
-0.152 MgHCO3+ 5.761e-005 4.211e-005 -4.239 -4.376 Mn(2) 3.951e-007 Mn+2 2.230e-007 5.922e-008 -6.652 -7.228 -0.136 Mn(2) 3.951e-007 Mn+2 2.230e-007 5.922e-008 -6.652 -7.228 -0.576 Mn+2 2.230e-007 7.562e-008 -6.685 -7.121					-0.136	-	3.346e-010	2.445e-010	-9.475	-9.612
-0.136 -0.576 -0	-0.152						2.230e-007	5.922e-008	-6.652	-7.228
	-0.136	_			-0.576					
	0.041				-0.136					

136	MnCl+	5.147e-008		-7.288	-7.425			or 1 -		oles i
41	Mn904	1.390e-008		-7.857	-7.816	Delta	Phase	SI 10g 1	AP log KT	Initi
41	MnC12	2.331e-009		-8.632	-8.592	5 504 005	02 (g)	-0.79 -3.	.68 –2.89 1	L.000e+0
41	Mh003		8.551e-010	-9.109	-9.068	6.591e-007				
L36	MnCl3-	1.504e-010		-9.823	-9.959			Solution com	osition	
136	MnCH+	5.585e-013	4.082e-013	-12.253	-12.389		Elements	Molality	Moles	
3)	4.555e-017 Mn+3	4.555e-017	2.709e-018	-16.342	-17.567		C		1.389e-001	
26	4.183e-004						Ca Cl	2.367e-001	1.476e-001 2.367e-001	
L46	Na+	4.132e-004	2.951e-004	-3.384	-3.530		Fe_di Fe_tri		4.531e-008 1.610e-004	
.36	NaS04-	2.934e-006	2.144e-006	-5.533	-5.669		K Mg	5.270e-005 9.719e-004	5.270e-005 9.719e-004	
1	NaHCO3		2.377e-006	-5.665	-5.624		Min Na	4.183e-004	3.951e-007 4.183e-004	
36	NaCO3-	1.367e-009	9.987e-010	-8.864	-9.001		S	1.579e-002	1.579e-002	
1	NaCH	4.760e-013	5.227e-013	-12.322	-12.282			-Description of	E solution	
	3.828e-004 02	1.914e-004	2.102e-004	-3.718	-3.677			ηΉ	= 5.432	Chan
L	0.000e+000					equilibrium		pe	= 15.170	Adju
	H2S	0.000e+000	0.000e+000	-137.957	-137.917	CQLIIII.	Act	ivity of water Ionic strength	= 0.991 = 4.066e-0	001
7	HS-	0.000e+000	0.000e+000	-139.239	-139.426		Mass	of water (kg) linity (eq/kg)	= 1.000e+0	000
	S-2	0.000e+000	0.000e+000	-146.277	-146.912		Tota	1 002 (mol/kg)	= 1.389e-(001
	Fe_di(HS)2	0.000e+000	0.000e+000	-276.293	-276.252	Denverse	Electrica	rature (deg C) 1 balance (eg)	= 3.342e-0	013
5	Fe_di (HS) 3-	0.000e+000	0.000e+000	-413.505	-413.641	Percent em	or, 100*(Cat- A	Iterations	= 0.00 = 92 = 1.1104214	-1000
	1.579e-002	0.017 000	1 010 000	0.005	1 005				= 1.110421e = 5.587731e	
	Ca904		1.012e-002	-2.035	-1.995			-Distribution o	of species-	
	904-2	6.491e-003		-2.188	-2.839					_
	MgSO4	7.774e-005		-4.109	-4.069	Log				Log
	NaSO4-		2.144e-006	-5.533	-5.669	Gamma.	Species	Molality	Activity	Molalit
	H904-	7.129e-007	5.210e-007	-6.147	-6.283		H+	4.791e-006	3.697e-006	-5.32
	K904-	4.794e-007	3.504e-007	-6.319	-6.455	-0.113	OH-		2.684e-009	-8.38
	CaHSO4+	2.999e-007	2.192e-007	-6.523	-6.659	-0.187	H2O		9.911e-001	1.74
	Fe_dis04	1.049e-007	1.152e-007	-6.979	-6.938	0.000 C(-4)	0.000e+000		001	
	Fe_triSO4+	1.556e-008	1.137e-008	-7.808	-7.944	0.041	CH4	0.000e+000	0.000e+000	-141.38
	Mn904	1.390e-008	1.527e-008	-7.857	-7.816	C(4)	1.389e-001 002	1.094001	1.201e-001	-0.96
	Fe_tri(SO4)2-	4.935e-010	3.607e-010	-9.307	-9.443	0.041	H003-		1.433e-002	-1.69
	Fe_diH904+	3.831e-012	2.800e-012	-11.417	-11.553	-0.152	CaHCO3+		6.396e-003	-2.04
	Fe_triHSO4+2	3.945e-013	1.125e-013	-12.404	-12.949	-0.152	MgHCO3+		4.210e-005	-4.23
		—Saturation i	ndicee			-0.136	CaCO3		1.068e-005	-5.01
		auduui 1				0.041			2.377e-006	-5.66
	Phase	SI log I	AP log KT			0.041	NaHCO3			
	Anhydrite	0.07 -4.				-0.610	003-2 Metron2		1.818e-007	-6.131
	Aragonite Calcite	0.14 -8. 0.28 -8.	20 -8.48	CaCO3		-0.136	MnHC03+		7.562e-008	-6.985 7.40
	CH4 (g) CO2 (g)	-138.48 -141. 0.55 -0.	92 -1.47	CCC2		0.041	MgCO3		4.356e-008	-7.40
	Dolomite Gypsum	-1.45 -18. 0.28 -4.	30 -4.58	CaMg(CO3)2 CaSO4:2H2C		-0.136	Fe_diH003+		1.082e-008	-7.830
	H2 (g) H2O(g)	-41.21 -44. -1.51 -0.	00 1.51			-0.136	NaCO3-		9.986e-010	-8.86
	H2S(g) Halite	-136.92 -137. -5.92 -4.	34 1.58	NaCl		0.041	MnCO3		8.550e-010	-9.10
	Hausmannite Manganite	-8.93 52. -1.11 24.	23 25.34	MnOOH		0.041	Fe_di003	2.999e-011	3.293e-011	-10.52
	02(g) Pyrochroite	-0.78 -3. -11.57 3.	68 –2.89 63 15.20	O2 Mn(OH)2		Ca	1.476e-001 Ca+2	1.293e-001	3.499e-002	-0.88
	Pyrolusite Rhodochrosite	3.45 44. -2.84 -13.	83 41.38 97 -11.13	MhC03		-0.568	CaSO4		1.012e-002	-2.03
	Sulfur	-101.59 -96.	71 4.88	S		0.041	CaHCO3+		6.396e-003	-2.04
ste	p 7.					-0.152	CaCO3		1.068e-005	-5.01
Ele	ment Fe <u>di</u> has no Enroneous mole					0.041	CaHSO4+		2.192e-007	-6.52
s.	Usually caused					-0.136	CaOH+		1.557e-009	-8.67
on.	May be due to 1					-0.136 Cl	2.367e-001	2.1300-009	1.55/6-005	0.07.
	r negative concer on 1.	ntrations in t	he diffuse :	layer.		-0.181	C1-	2.367e-001	1.559e-001	-0.62
e p	hase assemblage 1		od in aii	tion ?			MnCl+	5.147e-008	3.761e-008	-7.28
		Cinetics defin		LLIGH Z.		-0.136	Fe_triCl+2	1.200e-008	3.424e-009	-7.92
1.	Kinetics define				0 7.	-0.545	Fe_triCl2+	3.263e-009	2.385e-009	-8.48
	Time step: 8640					-0.136	MnC12	2.331e-009	2.560e-009	-8.63
ent	Rate name	Delta Moles	uotal Moles	Reactant		0.041	Fe_diCl+	2.224e-009	1.625e-009	-8.65
	Fe_di_ax	-2.636e-006	9.998e-001	Fe_di		-0.136	MnCl3-	1.504e-010	1.099e-010	-9.82
				Fe_tri		-0.136	Fe_triCl3		3.718e-011	-10.47
						0.041				
						0.041 Fe_di	4.531e-008			

	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
-0.136	Fe dis04	1.773e-009	1.947e-009	-8.751	-8.711
0.041	Fe diCO3	2.999e-011	3.293e-011	-10.523	-10.482
0.041	Fe_diOH+	8.763e-013	6.404e-013	-12.057	-12.194
-0.136	Fe diHSO4+	6.474e-014	4.732e-014	-13.189	-13.325
-0.136	Fe_di(HS)2	0.000e+000	0.000e+000	-278.065	-278.024
0.041	Fe_di(HS)3-	0.000e+000	0.000e+000	-415.277	-415.413
-0.136 Fe_tri	1.610e-004				
-0.136	Fe_tri(OH)2+	1.530e-004	1.118e-004	-3.815	-3.952
-0.545	Fe_triOH+2	4.414e-006	1.259e-006	-5.355	-5.900
0.041	Fe_tri(OH)3	3.516e-006	3.861e-006	-5.454	-5.413
-0.136	Fe_trisO4+	1.582e-008	1.156e-008	-7.801	-7.937
-1.226	Fe_tri+3	1.223e-008	7.273e-010	-7.913	-9.138
-0.545	Fe_triCl+2	1.200e-008	3.424e-009	-7.921	-8.465
-2.179	Fe_tri2(OH)2+4	6.442e-009	4.267e-011	-8.191	-10.370
-0.136	Fe_triCl2+	3.263e-009	2.385e-009	-8.486	-8.623
-3.405	Fe_tri3(OH)4+5	2.530e-009	9.966e-013	-8.597	-12.001
-0.136	Fe_tri(OH)4-	1.292e-009	9.442e-010	-8.889	-9.025
-0.136	Fe_tri(SO4)2-	5.018e-010	3.667e-010	-9.299	-9.436
0.041	Fe_triCl3	3.385e-011	3.718e-011	-10.470	-10.430
-0.545	Fe_triHSO4+2	4.012e-013	1.145e-013	-12.397	-12.941
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	3.440e-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	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	F 000 000	6 650	7 000
-0.576	Mn+2	2.230e-007	5.922e-008	-6.652	-7.228
-0.136	MnH003+	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	MnC12	2.331e-009 7.786e-010	2.560e-009 8.550e-010	-8.632	-8.592
0.041	MhCO3			-9.109	-9.068
-0.136	MnCl3-	1.504e-010	1.099e-010	-9.823	-9.959 12.300
-0.136	MnCH+	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	4.132e-004	2 051- 004	2 204	2 E20
-0.146	Na+ NaSO4-	2.934e-006	2.951e-004 2.144e-006	-3.384 -5.533	-3.530 -5.669
-0.136	NaHCO3	2.165e-006	2.377e-006	-5.665	-5.624
0.041	Nacos-	1.366e-009	9.986e-010	-8.864	-9.001
-0.136			5.227e-013	-12.322	
0.041	NaCH	4.760e-013	3.22/e-013	-12.322	-12.282
O(0) 0.041	3.828e-004 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		0.000e+000	0.000e+000	-139.239	-139.426
-0.187	HS- S-2	0.000e+000	0.000e+000	-139.239	-139.426
-0.635	5-2 Fe_di.(HS)2	0.000e+000	0.000e+000	-278.065	-278.024
0.041		0.000e+000	0.000e+000 0.000e+000	-278.065 -415.277	-278.024 -415.413
-0.136 g(6)	Fe_di(HS)3-	0.000e+000	v.uue+uu	-41J.Z//	-410.413
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 0.041	MgS04	7.774e-005	8.537e-005	-4.109	-4.069
0.041 -0.136	NaS04-	2.934e-006	2.144e-006	-5.533	-5.669

	HSO4-	7.130e-007 5.211e-007 -6.147 -6.283
-0.136	KSO4-	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		1.390e-008 1.527e-008 -7.857 -7.816
0.041	Fe dis04	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		
-0.545	Fe_triH904+2	
-0.136	Fe_diHSO4+	6.474e-014 4.732e-014 -13.189 -13.325
		-Saturation indices
	Phase	SI log IAP log KT
	CCI(g) Dolamite Oppsum H2(g) H2(g) H2S(g) H3lite Hausmarnite Merganite CCI(g) Pyrochroite Pyrolusite Pyrolusite	0.07 -4.29 -4.36 CaSM 0.14 -8.20 -8.34 CaSM 0.28 -8.20 -8.49 CaSM -138.48 -141.34 -2.86 CH 0.55 -0.92 -1.47 CO2 -1.45 -18.54 -17.09 Catg(CO3)2 -1.45 -18.54 -17.09 Catg(CO3)2 -41.21 -44.36 -3.15 H2 -1.51 -0.00 1.51 H20 -136.92 -137.92 -1.00 H2S -8.93 52.10 61.03 Mr304 -1.11 24.22 25.34 Mr30H -0.79 -3.68 -2.289 C2 -11.57 3.63 15.20 Mr1(CH)2 -3.44 31 41.38 Mr20 -2.84 -13.97 -11.13 Mr303
Reaction ste		-101.59 -96.71 4.88 S
	_	egative moles in solution, -2.872895e-008.
zero moles.		balance occurs as moles are added to produce
calculation.		by KINETICS, REACTION, or diffuse layer
	May be due to 1	arge time steps in early part of KINETICS
WARNING: Ele	ment Fe_di has ne	ntrations in the diffuse layer. gative moles in solution, -1.971399e-009. balance occurs as moles are added to produce
zero moles.		by KINETICS, REACTION, or diffuse layer
calculation.	_	
	r negative concer r negative concer ment Fe_di has na Erroneous mole	arge time steps in early part of KINETICS strations in the diffuse layer. gative moles in solution, -3.030945e-009. balance occurs as moles are added to produce
zero moles.		by KINETICS, REACTION, or diffuse layer
calculation. simulation of WARNING: Ele	May be due to l r negative concer	arge time steps in early part of KINETICS strations in the diffuse layer. agative moles in solution, -2.415059e-009.
zero moles.	Erroneous mole	balance occurs as moles are added to produce
calculation.		by KINETICS, REACTION, or diffuse layer
simulation o	ment Fe_di has ne	arge time steps in early part of KINETICS strations in the diffuse layer. spative moles in solution, -1.478622e-009.
zero moles.		balance occurs as moles are added to produce
calculation.		by KINETICS, REACTION, or diffuse layer
simulation of WARNING: Ele	r negative concer ment Fe_di has ne	arge time steps in early part of KINETICS strations in the diffuse layer. agative moles in solution, -7.499156e-010. balance occurs as moles are added to produce
zero moles.	Usually caused	by KINETICS, REACTION, or diffuse layer
calculation.	_	
WARNING: Ele	ment Fe_di has ne	arge time steps in early part of KINETICS strations in the diffuse layer. gative moles in solution, -3.589512e-011. balance occurs as moles are added to produce
zero moles.	Usually caused	by KINETICS, REACTION, or diffuse layer
calculation.	May be due to 1	arge time steps in early part of KINETICS
Using soluti	r negative concer on 1. hase assemblage 1	strations in the diffuse layer.
Kinetics 1.	Kinetics define	d in simulation 2.
	Time step: 1728	100 seconds (Incremented time: 345600 seconds)
Coefficient	Rate name	Delta Moles Total Moles Reactant
wermment	Fe_di_ox	-4.530e-008 9.998e-001 Fe_di
-1	. <u> </u>	-4.330e-006 9.996e-001 Fe_tri
1		te_tt
		Phase assemblage
		M-1
Delta	Phase	Moles in assemblage SI log IAP log KT Initial Final

O2 (g)

-0.78 -3.68 -2.89 1.000e+001 1.000e+001-

		-Solution com	osition			0.041	Fe_diCO3		9.436e-015	-14.066	-14.025
	_		_			-0.136			1.835e-016	-15.600	-15.736
	Elements	Molality	Moles			-0.136			1.356e-017	-16.732	-16.868
	C Ca	1.476e-001	1.389e-001 1.476e-001			0.041	Fe_di_(HS)2		0.000e+000	-281.608	-281.567
	Cl Fe_di	1.298e-011	2.367e-001 1.298e-011			-0.136			0.000e+000	-418.820	-418.956
	Fe_tri K	5.270e-005	1.610e-004 5.270e-005			Fe_tri	Fe_tri(OH)2		1.118e-004	-3.815	-3.951
	Mg Mn	3.951e-007	9.719e-004 3.951e-007			-0.136	Fe_triOH+2	4.415e-006	1.259e-006	-5.355	-5.900
	Na S		4.183e-004 1.579e-002			-0.545	Fe_tri(OH)3	3.517e-006	3.862e-006	-5.454	-5.413
		Description of	solution			0.041	Fe_tri504+	1.583e-008	1.157e-008	-7.801	-7.937
			F 422	G		-0.136 -1.226	Fe_tri+3	1.223e-008	7.275e-010	-7.913	-9.138
owillibrium		рн ре	= 5.432 = 15.170		e balance sed to redox	-0.545	Fe_triCl+2	1.201e-008	3.425e-009	-7.921	-8.465
equilibrium		vity of water		1		-2.179	Fe_tri2(OH)	2+4 6.446e-009	4.269e-011	-8.191	-10.370
	Mass	ofwater (kg)	= 4.066e-001 = 1.000e+000)		-2.179 -0.136	Fe_triCl2+	3.264e-009	2.385e-009	-8.486	-8.622
	Total	inity (eg/kg) CO2 (mol/kg)	= 2.983e-002 = 1.389e-002 = 25.000	1		-3.405	Fe_tri3(OH)	4+5 2.532e-009	9.974e-013	-8.597	-12.001
Descript con		ature (deg C) balance (eg)	= -1.264e-009	9		-0.136	Fe_tri(OH)4	l- 1.292e-009	9.444e-010	-8.889	-9.025
rescent est	or, 100" (cat- A1	Iterations		200			Fe_tri(SO4)	2- 5.020e-010	3.668e-010	-9.299	-9.436
		Total O	= 1.110421e+0 = 5.587731e+0	001		-0.136	Fe_triCl3	3.386e-011	3.719e-011	-10.470	-10.430
		Distribution o	of species			0.041	Fe_triH904+	+2 4.013e-013	1.145e-013	-12.397	-12.941
				T	T	-0.545 H(0)	0.000e+00	0 000000	0.000e+000	44.300	44 355
Log	ai	36-7-74	3-4-4 3	Log	Log	0.041	H2		0.000e+000	-44.396	-44.355
Gamma	Species	Molality	Activity N	olality	ACCIVITY	K	5.270e-00 K+	5.222e-005	3.440e-005	-4.282	-4.463
0.112	H+	4.791e-006	3.697e-006	-5.320	-5.432	-0.181	K904-	4.794e-007	3.504e-007	-6.319	-6.455
-0.113	OH-	4.133e-009	2.684e-009	-8.384	-8.571	-0.136	KOH	2.912e-014	3.198e-014	-13.536	-13.495
-0.187	H2O	5.551e+001	9.911e-001	1.744	-0.004	0.041 Mg	9.719e-00		0 F10- 004	2 070	3 (00
0.000 C(-4)	0.000e+000	0.000 .000	0.000 .000	141 204	141 242	-0.522			2.512e-004	-3.078	-3.600
0.041	CH4	0.000e+000	0.000e+000 -	-141.384	-141.343	0.041	MgS04		8.537e-005	-4.109	-4.069
C(4)	1.389e-001 cc2	1.094e-001	1.201e-001	-0.961	-0.920	-0.136			4.210e-005	-4.239	-4.376
0.041	H003-	2.035e-002	1.433e-002	-1.691	-1.844	0.041	MgC03		4.356e-008	-7.402	-7.361
-0.152	CaHOO3+	9.085e-003	6.396e-003	-2.042	-2.194	-0.136			2.445e-010	-9.476	-9.612
-0.152	MgHOO3+	5.761e-005	4.210e-005	-4.239	-4.376	Mn(2)	3.951e-00 Mn+2		5.922e-008	-6.652	-7.228
-0.136	CaCO3	9.729e-006	1.068e-005	-5.012	-4.971	-0.576	MnH003+	1.035e-007	7.562e-008	-6.985	-7.121
0.041	NaHCO3	2.165e-006	2.377e-006	-5.665	-5.624	-0.136	MnCl+	5.147e-008	3.761e-008	-7.288	-7.425
0.041	003-2	7.400e-007	1.818e-007	-6.131	-6.741	-0.136	Mn904	1.390e-008	1.527e-008	-7.857	-7.816
-0.610	MnHCO3+	1.035e-007	7.562e-008	-6.985	-7.121	0.041	MnCl2	2.331e-009	2.560e-009	-8.632	-8.592
-0.136 0.041	MgCCC3	3.967e-008	4.356e-008	-7.402	-7.361	0.041	MnC03	7.786e-010	8.550e-010	-9.109	-9.068
	NaCO3-	1.366e-009	9.986e-010	-8.864	-9.001		MnCl3-	1.504e-010	1.099e-010	-9.823	-9.959
-0.136 0.041	Mh003	7.786e-010	8.550e-010	-9.109	-9.068	-0.136 -0.136	MnCH+	5.585e-013	4.082e-013	-12.253	-12.389
-0.136	Fe_diH003+	4.243e-012	3.101e-012	-11.372	-11.509	Mn(3)	4.555e-01 Mn+3	17	2.710e-018	-16.341	-17.567
0.041	Fe_di003	8.593e-015	9.436e-015	-14.066	-14.025	-1.226 Na	4.183e-00		2.7100 010	10.541	17.507
Ca	1.476e-001 Ca+2	1 203 001	3.499e-002	-0.888	-1.456	-0.146	Na+		2.951e-004	-3.384	-3.530
-0.568	CaSO4		1.012e-002	-2.035	-1.995	-0.136	NaSO4-	2.934e-006	2.144e-006	-5.533	-5.669
0.041	CaHCO3+		6.396e-003	-2.042	-2.194	0.041	NaHOO3	2.165e-006	2.377e-006	-5.665	-5.624
-0.152	CaCO3		1.068e-005	-5.012	-4.971	-0.136	Nacco3-	1.366e-009	9.986e-010	-8.864	-9.001
0.041	CaHSO4+		2.192e-007	-6.523	-6.659	0.041	NaCH	4.760e-013	5.227e-013	-12.322	-12.282
-0.136	CaOH+		1.557e-009	-8.672	-8.808	0(0)	3.828e-00 02		2.102e-004	-3.718	-3.677
-0.136 Cl	2.367e-001			2.0.2	2.000	0.041 S(-2)	0.000e+00			3.,10	3.0.7
-0.181	C1-	2.367e-001	1.559e-001	-0.626	-0.807	0.041	H2S		0.000e+000	-137.957	-137.917
-0.136	MnCl+	5.147e-008	3.761e-008	-7.288	-7.425	-0.187	HS-	0.000e+000	0.000e+000	-139.239	-139.426
-0.545	Fe_triCl+2	1.201e-008	3.425e-009	-7.921	-8.465	-0.635	S-2	0.000e+000	0.000e+000	-146.277	-146.912
-0.136	Fe_triCl2+	3.264e-009	2.385e-009	-8.486	-8.622	0.041	Fe_di(HS)2	0.000e+000	0.000e+000	-281.608	-281.567
0.041	MhCl2	2.331e-009	2.560e-009	-8.632	-8.592	-0.136	Fe_di(HS)3-	0.000e+000	0.000e+000	-418.820	-418.956
-0.136	MnCl3-	1.504e-010	1.099e-010	-9.823	-9.959	S(6)	1.579e-00 CasO4		1.012e-002	-2.035	-1.995
0.041	Fe_triCl3	3.386e-011	3.719e-011	-10.470	-10.430	0.041	S04-2		1.450e-003	-2.188	-2.839
-0.136	Fe_diCl+	6.373e-013	4.658e-013	-12.196	-12.332	-0.651			8.537e-005	-4.109	-4.069
Fe_di	1.298e-011 Fe_di+2	7.587 <u>–</u> 012	2.164e-012	-11.120	-11.665	0.041	NaSO4-		2.144e-006	-5.533	-5.669
-0.545	Fe_diH003+			-11.372	-11.509	-0.136			5.211e-007	-6.147	-6.283
-0.136	re_dicl+			-12.196	-12.332	-0.136			3.504e-007	-6.319	-6.455
-0.136	Fe_dis04			-12.190	-12.253	-0.136			2.192e-007	-6.523	-6.659
0.041		5.0010-013	J.J.W. VIJ	4√نه، سد		-0.136		2.222007	2.122-007	دعد، ن	0.003

-0.136	Fe_triSO4+	1.583e-008	1.157e-008	-7.801	-7.937	1	C Ca	1.389e-001 1.476e-001	1.389e-001		
0.041	MnSO4	1.390e-008	1.527e-008	-7.857	-7.816		Cl Fe_di	2.367e-001 3.720e-015	2.367e-001		
-0.136	Fe_tri(SO4)2-	5.020e-010	3.668e-010	-9.299	-9.436		Fe_tri K	1.610e-004 5.270e-005	1.610e-004		
0.041	Fe_dis04	5.081e-013	5.580e-013	-12.294	-12.253		Mg Mn	9.719e-004 3.951e-007	9.719e-004		
-0.545	Fe_triHSO4+2	4.013e-013	1.145e-013	-12.397	-12.941		Na S	4.183e-004 1.579e-002	4.183e-004		
-0.136	Fe_diH904+	1.855e-017	1.356e-017	-16.732	-16.868			-Description of			
		—Saturation i	ndices							_	
	M	OT 1 T	3D 1 18TD					pH pe	= 5.432 = 15.170		e balance ed to redox
	Phase Arhydrite Aragonite Calcite CH4(g) CD2(g) Dolomite Gypsum H2(g) H2O(g) HSS(g) Halite	0.07 -4. 0.14 -8. 0.28 -8. -138.48 -141. 0.55 -0. -1.45 -18. 0.28 -4. -41.21 -44. -1.51 -0. -136.92 -137. -5.92 -4.	20 -8.34 20 -8.48 34 -2.86 92 -1.47 54 -17.09 30 -4.58 36 -3.15 00 1.51 92 -1.00	CaCO3 CaCO3 CH4 CO2 CaMg(CO3)2 CaSO4:2H2O H2 H2O H2O H2S		equilibrium Percent en	Mass Total alka Tota Tempe	Iterations	= 4.066e-(= 1.000e+(= 2.983e-(= 1.389e-(= 25.000 = -1.265e-(= -0.00	000 002 001 009	
	Hausmannite Manganite	-8.93 52. -1.11 24.	10 61.03 23 25.34					-Distribution o	of species		
	02(g) Pyrochroite	-0.78 -3. -11.57 3.	68 –2.89 63 15.20	O2 Mn (OH) 2						Log	Log
	Pyrolusite Rhodochrosite Sulfur	3.45 44. -2.84 -13. -101.59 -96.	97 -11.13	MnCO3		Log Gamma	Species	Molality	Activity	Molality	Activity
Reaction ste	p 9.					-0.113	H+	4.791e-006	3.697e-006	-5.320	-5.432
WARNING: Ele	ment Fe_di has n Enroneous mole					-0.113	OH-	4.133e-009	2.684e-009	-8.384	-8.571
zero moles.	Usually caused					0.000	H2O	5.551e+001	9.911e-001	1.744	-0.004
calculation.		arge time ste	ps in early	part of KII	-	C(-4) 0.041	0.000e+000 CH4	0.000e+000	0.000e+000	-141.384	-141.343
WARNING: Ele	ment Fe_di has n Erroneous mole	egative moles balance occur	in solution s as moles a	, -5.648819 are added to	e-013. o produce	C(4)	1.389e-001 co2	1.094e-001	1.201e-001	-0.961	-0.920
zero moles.	Usually caused	by KINETICS,	REACTION, O	r diffuse la	ayer	0.041	H003-	2.035e-002	1.433e-002	-1.691	-1.844
calculation.	May be due to 1	arge time ste	ps in early	part of KII	ETICS	-0.152	CaH003+	9.085e-003	6.396e-003	-2.042	-2.194
	or negative conce ment Fe_di has n	egative moles	in solution	, -8.685081		-0.152	MgHCO3+	5.761e-005	4.210e-005	-4.239	-4.376
zero moles.	Erroneous mole					-0.136	CaCO3	9.729e-006	1.068e-005	-5.012	-4.971
calculation.						0.041	NaHCO3	2.165e-006	2.377e-006	-5.665	-5.624
simulation o	May be due to I or negative conce	ntrations in t	he diffuse i	layer.		0.041	003-2	7.400e-007	1.818e-007	-6.131	-6.741
	ment Fe_di has n Enroneous mole					-0.610	MnH003+	1.035e-007	7.562e-008	-6.985	-7.121
zero moles.	Usually caused	by KINETICS,	REACTION, O	r diffuse la	ayer	-0.136	MgCO3	3.967e-008	4.356e-008	-7.402	-7.361
calculation.	May be due to 1	arge time ste	ps in early	part of KII	NETICS	0.041	NaCO3-	1.366e-009	9.986e-010	-8.864	-9.001
	or negative conce ment Fe_di has n	egative moles	in solution	, -4.236973	e-013.	-0.136	MnCO3	7.786e-010	8.550e-010	-9.109	-9.068
zero moles.	Erroneous mole				_	0.041	Fe_diH003+	1.216e-015	8.885e-016	-14.915	-15.051
calculation.						-0.136	Fe_diCO3	2.462e-018	2.704e-018	-17.609	-17.568
simulation o	May be due to l or negative concer	ntrations in t	he diffuse i	layer.		0.041 Ca	1.476e-001	1.293e-001	2 400 000	0.000	1 456
zero moles.	ment Fe_di has n Enroneous mole					-0.568	Ca+2 CaSO4	9.217e-003		-0.888 -2.035	-1.456 -1.995
calculation.	Usually caused	by KINETICS,	REACTION, or	r diffuse la	ayer	0.041	CaHOO3+	9.085e-003		-2.033	-2.194
	May be due to l or negative conce	large time ste	ps in early	part of KII	ETICS	-0.152	CaCO3	9.729e-006		-5.012	-4.971
	ment Fe_di has n Erroneous mole	egative moles	in solution	, -1.028570	e-014.	0.041	CaHSO4+	2.999e-007		-6.523	-6.659
zero moles.	Usually caused				_	-0.136	CaOH+	2.130e-009		-8.672	-8.808
calculation.		_			_	-0.136 Cl	2.367e-001				
simulation o Using soluti	or negative conce					-0.181	Cl-	2.367e-001	1.559e-001	-0.626	-0.807
	hase assemblage :	l. Tinetics defin	ed in simula	ation 2.		-0.136	MnCl+	5.147e-008	3.761e-008	-7.288	-7.425
	Kinetics define					-0.545	Fe_triC1+2	1.201e-008	3.425e-009	-7.921	-8.465
	Time step: 1728			time: 51840	00 seconds)	-0.136	Fe_triCl2+	3.264e-009	2.385e-009	-8.486	-8.622
	Rate name	Delta Moles				0.041	MnCl2	2.331e-009		-8.632	-8.592
Coefficient						-0.136	MnCl3-		1.099e-010	-9.823	-9.959
-1	Fe_di_ax	-1.298e-011	9.998e-001			0.041	Fe_triCl3	3.386e-011		-10.470	-10.430
1				Fe_tri		-0.136	Fe_diCl+	1.826e-016	1.335e-016	-15.738	-15.875
		Phase assen	iblage			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
_	Phase	SI log I	AP log KT	Moles in as Initial	semblage Final	-0.136	Fe_diCl+	1.826e-016	1.335e-016	-15.738	-15.875
Delta	****	0.05				-0.136	Fe_disO4	1.456e-016	1.599e-016	-15.837	-15.796
3.196e-012	02 (g)	-0.78 -3.	68 –2.89	L.000e+001 1	L.000e+001-	0.041	Fe_di003	2.462e-018	2.704e-018	-17.609	-17.568
		-Solution comp	osition			0.041	Fe_diOH+	7.195e-020	5.258e-020	-19.143	-19.279
						-0.136	Fe_diHSO4+	5.316e-021	3.885e-021	-20.274	-20.411
	Elements	Molality	Moles			-0.136					

0.041	Fe_di (HS)2	0.000e+000	0.000e+000	-285.150	-285.110
-0.136	Fe_di (HS) 3-	0.000e+000	0.000e+000	-422.363	-422.499
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	Fe_triSO4+	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_triC1+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 -3.405	Fe_tri3(OH)4+5	2.532e-009	9.974e-013	-8.597	-12.001
-3.405 -0.136	Fe_tri(OH)4-	1.292e-009	9.444e-010	-8.889	-9.025
	Fe_tri(SO4)2-	5.020e-010	3.668e-010	-9.299	-9.436
-0.136 0.041	Fe_triCl3	3.386e-011	3.719e-011	-10.470	-10.430
-0.545	Fe_triH904+2	4.013e-013	1.145e-013	-12.397	-12.941
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	3.440e-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	MgHCO3+	5.761e-005	4.210e-005	-4.239	-4.376
-0.136	MgC03	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 Mn+2	2.230e-007	5.922e-008	-6.652	-7.228
-0.576	MnHCO3+	1.035e-007	7.562e-008	-6.985	-7.121
-0.136	MnCl+	5.147e-008	3.761e-008	-7.288	-7.425
-0.136	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	MnCO3	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	4.555e-017	2.710e-018	16 241	17 507
-1.226 Na	Mn+3 4.183e-004	4.555e-01/	2.710e-018	-16.341	-17.567
-0.146	1.165E-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
0.041	NaHOO3	2.165e-006	2.377e-006	-5.665	-5.624
-0.136	NaCO3-	1.366e-009	9.986e-010	-8.864	-9.001
0.041	NaOH	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
0.041 S(-2)	0.000e+000	0.000e+000	0.000e+000	-137.957	-137.917
0.041	H2S HS-	0.000e+000	0.000e+000	-137.957	-137.917
-0.187	S-2	0.000e+000	0.000e+000	-139.239	-139.420
-0.635	S-2 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	0.000e1000	0.00000	-422.303	-422.499
0.041	CaSO4	9.217e-003	1.012e-002	-2.035	-1.995
-0.651	SO4-2	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
-0.136	HS04-	7.130e-007	5.211e-007	-6.147	-6.283
	KSO4-	4.794e-007	3.504e-007	-6.319	-6.455
-0.136 0.136	CaHSO4+	2.999e-007	2.192e-007	-6.523	-6.659
-0.136	Fe_triSO4+	1.583e-008	1.157e-008	-7.801	-7.937
-0.136	Mn904	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
-0.136					

-0.545	Fe_triH904+2	4.013e-013	1.145e-013	-12.397	-12.941
0.041	Fe_dis04	1.456e-016	1.599e-016	-15.837	-15.796
-0.136	Fe_diHSO4+	5.316e-021	3.885e-021	-20.274	-20.411
		—Saturation i	indices		
	Phase	CT lor I	AP log KT		
	Anhydrite	0.07 -4.	_	Ca904	
	Aragonite Calcite	0.14 -8. 0.28 -8.	20 -8.34 20 -8.48	CaCCC3 CaCCC3	
	CO2 (g)	-138.48 -141. 0.55 -0. -1.45 -18.	92 -1.47	CH4 CO2	
	Dolomite Gypsum H2(g)	0.28 -4. -41.21 -44.	30 -4.58	CaMg(CO3)2 CaSO4:2H2O H2	
	H2O(g)	-1.51 -0. -136.92 -137.	00 1.51 92 -1.00	H2O H2S	
	Halite Hausmannite	-5.92 -4. -8.93 52.	10 61.03	Mn304	
	Manganite 02(g) Pyrochroite	-1.11 24. -0.78 -3. -11.57 3	68 -2.89	02	
	Pyrolusite Rhodochrosite	-11.57 3. 3.45 44. -2.84 -13.	83 41.38	MnO2 MnCO3	
	Sulfur	-101.59 -96.			
Reaction step		ventire molecu	in colution	2 250017	015
zero moles.	ment Fe_di has ne Enroneous mole				
calculation.	Usually caused				
simulation o	May be due to 1 negative concer	arge time ste trations in t	ps in early he diffuse	part of KIN layer.	ETICS
WARNING: Eler zero moles.	ment Fe_di has ne Erroneous mole				
calculation.	Usually caused				
simulation o	May be due to 1 negative concer	arge time ste trations in t	ps in early he diffuse	part of KIN layer.	ETICS
WARNING: Eler zero moles.	ment Fe_di has ne Erroneous mole	gative moles balance occur	in solution s as moles	, -2.488/00e are added to	÷016. produce
calculation.	Usually caused	by KINETICS,	REACTION, O	r diffuse la	yer .
	May be due to 1 negative concer	arge time ste strations in t	ps in early he diffuse	part of KIN layer.	ETICS
	negative concer ment Fe di has ne Erroneous mole	gative moles balance occur	in solution s as moles	, -1.983007e are added to	÷016. produce
zero moles. calculation.	Usually caused	by KINETICS,	REACTION, o	r diffuse la	iyer
simulation on WARNING: Eler	May be due to l r negative concer ment Fe_di has no Enroneous mole	gative moles	in solution	, −1.214100∈	- 016.
zero moles. calculation.	Usually caused	by KINETICS,	REACTION, O	r diffuse la	iyer
simulation o	May be due to l negative concer ment Fe_di has ne	strations in t gative moles	he diffuse in solution	layer. , -6.157574e	- 017.
zero moles.	Erroneous mole Usually caused				
calculation.					
simulation on WARNING: Eler	May be due to l negative concer nent Fe_di has ne	gative moles	in solution	, -2.94/35/e	e-018.
zero moles.	Erroneous mole Usually caused				_
calculation.	_	_			_
Usina solutia	nase assemblace 1				
	Kinetics define				
	Time step: 1728	00 seconds (Incremented	time: 69120	10 seconds)
Coefficient	Rate name	Delta Moles	Total Moles	Reactant	
	Fe_di_ax	-3.886e-015	9.998e-001	Fe_di	
-1 1				Fe_tri	
		Phase assen	iblace		
Delta	Phase	SI log I	AP log KT	Moles in ass Initial	semblage Final
1.048e-013	O2 (g)	-0.78 -3.	68 –2.89	1.000e+001 1	000e+001
		Solution com	osition		
	Elements	Molality	Moles		
	С	1.389e-001	1.389e-001		
	Ca Cl Fe_di	0.007 001	1.476e-001 2.367e-001 1.066e-018		
	Fe_tri K	1.610e-004 5.270e-005	1.610e-004 5.270e-005		

	Mg Mn	9.719e-004 3.951e-007	9.719e-004 3.951e-007			-0.545	Fe_triOH+2	4.415e-006	1.259e-006	-5.355	-5.90
	Na S	4.183e-004 1.579e-002	4.183e-004			0.041	Fe_tri(OH)3	3.517e-006	3.862e-006	-5.454	-5.41
		Description of				-0.136	Fe_tri504+	1.583e-008	1.157e-008	-7.801	-7.93
						-1.226	Fe_tri+3	1.223e-008	7.275e-010	-7.913	-9.13
		pH pe	= 5.432 = 15.170		e balance ced to redox	-0.545	Fe_triCl+2	1.201e-008	3.425e-009	-7.921	-8.46
equilibrium	Acti	vity of water				-2.179	Fe_tri2(OH)2+4	6.446e-009	4.269e-011	-8.191	-10.37
	1	onic strength of water (kg)	= 4.066e-0 = 1.000e+0	000		-0.136	Fe_triCl2+	3.264e-009	2.385e-009	-8.486	-8.62
	Total alkal	inity (eg/kg) . CO2 (mol/kg)	= 2.983e-0 = 1.389e-0	002		-3.405	Fe_tri3(OH)4+5	2.532e-009	9.974e-013	-8.597	-12.00
	Electrical	ature (deg C) balance (eg)	= 25.000 = -1.265e-0	009		-0.136	Fe_tri(OH)4-	1.292e-009	9.444e-010	-8.889	-9.02
Percent erro	or, 100*(Cat- Ar	Iterations	= -0.00 = 233			-0.136	Fe_tri(SO4)2-		3.668e-010	-9.299	-9.43
		Total H Total O	= 1.110421e = 5.587731e	+002 +001		0.041	Fe_triCl3		3.719e-011	-10.470	-10.43
		Distribution o	of species			-0.545	Fe_triHSO4+2	4.013e-013	1.145e-013	-12.397	-12.94
				_	_	H(0)	0.000e+000 H2	0.000e+000	0.000e+000	-44.396	-44.35
Log	a .	26.7.77		Log	Log	0.041 K	5.270e-005	F 000 00F	2 440 005	4 000	4.40
Gamma.	Species	Molality	Activity	Molality	Activity	-0.181	K+		3.440e-005	-4.282	-4.46
0.113	H+	4.791e-006	3.697e-006	-5.320	-5.432	-0.136	K904-		3.504e-007	-6.319	-6.45
-0.113	OH-	4.133e-009	2.684e-009	-8.384	-8.571	0.041	KOH 0.710004	2.912 e -014	3.198e-014	-13.536	-13.49
-0.187	H2O	5.551e+001	9.911e-001	1.744	-0.004	Mg	9.719e-004 Mg+2	8.365e-004	2.512e-004	-3.078	-3.60
0.000 C(-4)	0.000e+000	0.000000	0.000-+000	141 204	141 242	-0.522	MgS04	7.774e-005	8.537e-005	-4.109	-4.06
0.041	CH4	v.uu0e+000	0.000e+000	-141.384	-141.343	0.041	MgHCO3+	5.761e-005	4.210e-005	-4.239	-4.376
C(4)	1.389e-001 CO2	1.094e-001	1.201e-001	-0.961	-0.920	-0.136	MgC03	3.967e-008	4.356e-008	-7.402	-7.36
0.041 -0.152	H003-	2.035e-002	1.433e-002	-1.691	-1.844	0.041 -0.136	MgCH+	3.346e-010	2.445e-010	-9.476	-9.612
-0.152 -0.152	CaHCO3+	9.085e-003	6.396e-003	-2.042	-2.194	Mn(2)	3.951e-007 Mn+2	2 220- 007	5.922e-008	-6.652	-7.228
	MgHCO3+	5.761e-005	4.210e-005	-4.239	-4.376	-0.576					-7.12
-0.136 0.041	CaCO3	9.729e-006	1.068e-005	-5.012	-4.971	-0.136	MnHCO3+ MnCl+		7.562e-008	-6.985 -7.288	-7.42
0.041	NaHCO3	2.165e-006	2.377e-006	-5.665	-5.624	-0.136	MnSO4		3.761e-008 1.527e-008	-7.200	-7.42. -7.81
-0.610	003-2	7.400e-007	1.818e-007	-6.131	-6.741	0.041	MnCl2			-8.632	-8.592
	MnHCO3+	1.035e-007	7.562e-008	-6.985	-7.121	0.041			2.560e-009	-9.109	
-0.136 0.041	MgC03	3.967e-008	4.356e-008	-7.402	-7.361	0.041	MnCO3 MnCl3-		8.550e-010 1.099e-010	-9.823	-9.066 -9.959
-0.136	NaCO3-	1.366e-009	9.986e-010	-8.864	-9.001	-0.136	MnOH+		4.082e-013	-12.253	-12.38
0.041	MhCO3	7.786e-010	8.550e-010	-9.109	-9.068	-0.136 Mn(3)	4.555e-017	3.363E-013	4.002E-015	-12.233	-12.30
-0.136	Fe_diH003+	3.484e-019	2.546e-019	-18.458	-18.594	-1.226	Mn+3	4.555e-017	2.710e-018	-16.341	-17.56
0.041	Fe_di003	7.056e-022	7.748e-022	-21.151	-21.111	Na.	4.183e-004 Na+	4 1320 004	2.951e-004	-3.384	-3.530
Ca	1.476e-001 Ca+2	1.293e-001	3 /1990_002	-0.888	-1.456	-0.146	NaSO4-		2.144e-006	-5.533	-5.66
-0.568	CaSO4	9.217e-003		-2.035	-1.995	-0.136	NaHCO3		2.377e-006	-5.665	-5.62
0.041	CaHOO3+	9.085e-003		-2.042	-2.194	0.041	NaCO3-		9.986e-010	-8.864	-9.001
-0.152	CaCO3		1.068e-005	-5.012	-4.971	-0.136	NaOH		5.227e-013	-12.322	-12.282
0.041	CaHSO4+	2.999e-007		-6.523	-6.659	0.041 O(0)	3.828e-004	117000 010	3,2270 023	11.511	111100
-0.136	CaOH+	2.130e-009		-8.672	-8.808	0.041	02	1.914e-004	2.102e-004	-3.718	-3.67
-0.136 Cl	2.367e-001	212300 003	113370 003	0.072	0.000	S(-2)	0.000e+000 H2S	0.000e+000	0.000e+000	-137.957	-137.917
-0.181	C1-	2.367e-001	1.559e-001	-0.626	-0.807	0.041	HS-		0.000e+000		-139.426
-0.136	MnCl+	5.147e-008	3.761e-008	-7.288	-7.425	-0.187	S-2		0.000e+000	-146.277	
-0.545	Fe_triCl+2	1.201e-008	3.425e-009	-7.921	-8.465	-0.635	Fe_di (HS)2		0.000e+000	-288.693	-288.653
-0.136	Fe_triCl2+	3.264e-009	2.385e-009	-8.486	-8.622	0.041	Fe_di (HS)3-		0.000e+000		
0.041	MnC12	2.331e-009	2.560e-009	-8.632	-8.592	-0.136 S(6)	1.579e-002				
-0.136	MnCl3-	1.504e-010	1.099e-010	-9.823	-9.959	0.041	CaSO4	9.217e-003	1.012e-002	-2.035	-1.995
0.041	Fe_triCl3	3.386e-011	3.719e-011	-10.470	-10.430	-0.651	904-2	6.491e-003	1.450e-003	-2.188	-2.839
-0.136	Fe_diCl+	5.233e-020	3.824e-020	-19.281	-19.417	0.041	MgS04	7.774e-005	8.537e-005	-4.109	-4.069
Fe_di	1.066e-018 Fe_di+2	6.230e-019	1.777e-019	-18.206	-18.750	-0.136	NaSO4-	2.934e-006	2.144e-006	-5.533	-5.669
-0.545	Fe_diHOO3+	3.484e-019		-18.458	-18.594	-0.136	H904-	7.130e-007	5.211e-007	-6.147	-6.28
-0.136	Fe_diCl+	5.233e-020		-19.281	-19.417	-0.136	KSO4-	4.794e-007	3.504e-007	-6.319	-6.45
-0.136	Fe_dis04	4.172e-020		-19.380	-19.339	-0.136	CaH904+	2.999e-007	2.192e-007	-6.523	-6.659
0.041	Fe_diCO3	7.056e-022		-21.151	-21.111	-0.136	Fe_trisO4+	1.583e-008	1.157e-008	-7.801	-7.93
0.041	Fe_diOH+	2.062e-023		-22.686	-22.822	0.041	MnSO4	1.390e-008	1.527e-008	-7.857	-7.81
-0.136	Fe_diHSO4+	1.523e-024		-23.817	-23.953	-0.136	Fe_tri(SO4)2-	5.020e-010	3.668e-010	-9.299	-9.43
-0.136	Fe_di(HS)2	0.000e+000		-288.693	-288.653	-0.545	Fe_triHSO4+2	4.013e-013	1.145e-013	-12.397	-12.94
0.041	Fe_di(HS)3-		0.000e+000	-425.906		0.041	Fe_diSO4	4.172e-020	4.582e-020	-19.380	-19.339
-0.136					· · · =	-0.136	Fe_diH904+	1.523e-024	1.113e-024	-23.817	-23.953
Fe_tri	1.610e-004										

	Saturation indices
	Phase SI log IAP log KT
	Anhydrite 0.07 -4.29 -4.36 CaSO4 Aragonite 0.14 -8.20 -8.34 CaCO3
	Calcite 0.28 -8.20 -8.48 CaCO3 CH4(g) -138.48 -141.34 -2.86 CH4
	CO2(g) 0.55 -0.92 -1.47 CO2 Dolamite -1.45 -18.54 -17.09 CaMg(CO3)2
	Gypsum 0.28 -4.30 -4.58 Cas04:2H20
	H2O(a) -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 Mn00H
	O2(g) -0.78 -3.68 -2.89 O2
	Pyrolusite 3.45 44.83 41.38 MnO2
	Rindochrosite -2.84 -13.97 -11.13 Mrc03 Sulfur -101.59 -96.71 4.88 S
Reaction step	o 11.
VARNING: Eler	ment Fe_di has negative moles in solution, -6.759450e-019.
zero moles.	Erroneous mole balance occurs as moles are added to produce
calculation.	Usually caused by KINETICS, REACTION, or diffuse layer
simulation o	May be due to large time steps in early part of KINEFICS r negative concentrations in the diffuse layer.
WARNING: Eler	ment Fe_di has negative moles in solution, -4.638259e-020. Enroneous mole balance occurs as moles are added to produce
zero moles.	Usually caused by KINETICS, REACTION, or diffuse layer
calculation.	
simulation o	May be due to large time steps in early part of KINETICS rnegative concentrations in the diffuse layer.
WARNING: Eler	ment Fe_di has negative moles in solution, -7.131341e-020. Ennoneous 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 rnegative concentrations in the diffuse layer.
simulation on WARNING: Eler	ment Fe_di has negative moles in solution, -5.682284e-020.
zero moles.	Erroneous mole balance occurs as moles are added to produce
calculation.	Usually caused by KINETICS, REACTION, or diffuse layer
simulation on WARNING: Eler	May be due to large time steps in early part of KINETICS range time steps in the diffuse layer. The step is the steps in the step in th
zero moles.	Erroneous mole balance occurs as moles are added to produce
calculation.	Usually caused by KINETICS, REACTION, or diffuse layer
	May be due to large time steps in early part of KINETICS rnegative concentrations in the diffuse layer.
WARNING: Eler	ment Fe_di has negative moles in solution, -1.764446e-020.
zero moles.	Erroneous mole balance occurs as moles are added to produce
calculation.	Usually caused by KINETICS, REACTION, or diffuse layer
WARNING: Eler	May be due to large time steps in early part of KINETICS r negative concentrations in the diffuse layer. nent Fe_di has negative moles in solution, -8.445617e-022. Exroneous 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 solutio	
Using kinetio	nase assemblage 1. es 1. Kinetics defined in simulation 2.
Kinetics 1.	Kinetics defined in simulation 2.
	Time step: 172800 seconds (Incremented time: 864000 seconds)
Doefficient	Rate name Delta Moles Total Moles Reactant
	Fe_di_ox 0.000e+000 9.998e-001 Fe_di
-1	Fe_tri
1	
	Phase assemblage
	Moles in assemblage
Delta	Phase SI log IAP log KT Initial Final
1.243e-013	C2(g) -0.78 -3.68 -2.89 1.000e+001 1.000e+001
	Solution composition
	Flamente Molslitz Molco
	Elements Molality Moles
	C 1.389e-001 1.389e-001 Ca 1.476e-001 1.476e-001
	Ca 1.476e-001 1.476e-001 Cl 2.367e-001 2.367e-001 Fe_dii 3.055e-022 3.055e-022
	Fe_tri 1.610e-004 1.610e-004
	K 5.270e-005 5.270e-005 Mg 9.719e-004 9.719e-004
	Mn 3.951e-007 3.951e-007 Na 4.183e-004 4.183e-004 S 1.579e-002 1.579e-002
	Mn 3.951e-007 3.951e-007 Na 4.183e-004 4.183e-004

pH = 5.432 pe = 15.170 Charge balance Adjusted to redox equilibrium

equilibrium

Activity of water = 0.991

Ionic strength = 4.066e-001

Mass of water (kg) = 1.000e+000

Total alkalimity (eg/kg) = 2.983e-002

Total CC (mol/kg) = 1.389e-001

Temperature (deg C) = 25.000

Electrical balance (eg) = -1.265e-009

Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.00

Iterations = 233

Total H = 1.110421e+002

Total O = 5.587731e+001

10tal 0 - 3.367/31e+001								
		Distribution o	of species					
				Log	Log			
Log	Species	Molality	Activity	Molality	Activity			
Gamma.								
-0.113	H+	4.791e-006	3.697e-006	-5.320	-5.432			
0.187	OH-	4.133e-009	2.684e-009	-8.384	-8.571			
.000	H2O	5.551e+001	9.911e-001	1.744	-0.004			
(-4)	0.000e+000 CH4	0.000e+000	0.000e+000	-141.384	-141.343			
.041 (4)	1.389e-001	1 004 001	1 001 001	0.001	0.000			
.041	002	1.094e-001	1.201e-001	-0.961	-0.920			
.152	H003-	2.035e-002	1.433e-002	-1.691	-1.844			
.152	CaH003+	9.085e-003	6.396e-003	-2.042	-2.194			
136	MgHCO3+	5.761e-005	4.210e-005	-4.239	-4.376			
11	CaCO3	9.729e-006	1.068e-005	-5.012	-4.971			
41	NaHCO3	2.165e-006	2.377e-006	-5.665	-5.624			
510	003–2	7.400e-007	1.818e-007	-6.131	-6.741			
136	MnHCO3+	1.035e-007	7.562e-008	-6.985	-7.121			
)41	MgCO3	3.967e-008	4.356e-008	-7.402	-7.361			
.136	NaCO3-	1.366e-009	9.986e-010	-8.864	-9.001			
041	MnCO3	7.786e-010	8.550e-010	-9.109	-9.068			
136	Fe_diH003+	9.982e-023	7.295e-023	-22.001	-22.137			
41	Fe_di003	2.022e-025	2.220e-025	-24.694	-24.654			
	1.476e-001 Ca+2	1.293e-001	3.499e-002	-0.888	-1.456			
568	CaSO4	9.217e-003	1.012e-002	-2.035	-1.995			
41	CaH003+	9.085e-003	6.396e-003	-2.042	-2.194			
152	CaCC3	9.729e-006	1.068e-005	-5.012	-4.971			
11	CaHSO4+	2.999e-007	2.192e-007	-6.523	-6.659			
136	CaOH+	2.130e-009	1.557e-009	-8.672	-8.808			
36	2.367e-001	21200 003	1.5570 005	0.072	0.000			
.81	C1-	2.367e-001	1.559e-001	-0.626	-0.807			
136	MnCl+	5.147e-008	3.761e-008	-7.288	-7.425			
545	Fe_triCl+2	1.201e-008	3.425e-009	-7.921	-8.465			
136	Fe_triCl2+	3.264e-009	2.385e-009	-8.486	-8.622			
41	MnCl2	2.331e-009	2.560e-009	-8.632	-8.592			
136	MnCl3-	1.504e-010	1.099e-010	-9.823	-9.959			
41	Fe_triCl3	3.386e-011	3.719e-011	-10.470	-10.430			
136	Fe_diCl+	1.500e-023	1.096e-023	-22.824	-22.960			
di	3.055e-022 Fe_di+2	1.785e-022	5.092e-023	-21.748	-22.293			
.545	Fe_diH003+	9.982e-023	7.295e-023	-22.001	-22.137			
.136	Fe_diCl+	1.500e-023	1.096e-023	-22.824	-22.960			
.136	Fe_dis04	1.196e-023	1.313e-023	-22.922	-22.882			
041		2.022e-025	2.220e-025	-24.694	-24.654			
041	Fe_dico3	5.908e-027						
.136	Fe_diOH+ Fe_diHSO4+		4.318e-027 3.190e-028	-26.229	-26.365			
.136	_	4.365e-028		-27.360	-27.496 -292.195			
041	Fe_di(HS)2	0.000e+000	0.000e+000	-292.236				
.136	Fe_di(HS)3-	0.000e+000	0.000e+000	-429.448	-429.585			
tri 126	1.610e-004 Fe_tri(OH)2+	1.530e-004	1.118e-004	-3.815	-3.951			
.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			
.041	Fe_triSO4+	1.583e-008	1.157e-008	-7.801	-7.937			
0.136								

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(OH)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 -0.545	Fe_triHSO4+2	4.013e-013	1.145e-013	-12.397	-12.941
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	3.440e-005	-4.282	-4.463
-0.136	KSO4-	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	Mg:904	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	Mgccc3	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 Mn+2	2.230e-007	5.922e-008	-6.652	-7.228
-0.576	MnH003+	1.035e-007	7.562e-008	-6.985	-7.121
-0.136	MnCl+	5.147e-008	3.761e-008	-7.288	-7.425
-0.136	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
0.041	MnC13-	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
-1.226 Na	4.183e-004				
-0.146	Na+	4.132e-004	2.951e-004	-3.384	-3.530
-0.136	NaSO4-	2.934e-006	2.144e-006	-5.533	-5.669
0.041	NaHCO3	2.165e-006	2.377e-006	-5.665	-5.624
-0.136	NaCO3-	1.366e-009	9.986e-010	-8.864	-9.001
0.041	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
0.041 S(-2)	0.000e+000				

0.041	H2S	0.000e+000	0.000e+000	-137.957	-137.917
****	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	-292.236	-292.195
0.041	Fe_di(HS)3-	0.000e+000	0.000e+000	-429.448	-429.585
-0.136 S(6)	1.579e-002 CaSO4	9.217e-003	1.012e-002	-2.035	-1.995
0.041	904-2	6.491e-003	1.450e-003	-2.188	-2.839
-0.651					
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
-0.136	HSO4-	7.130e-007	5.211e-007	-6.147	-6.283
-0.136	K904-	4.794e-007	3.504e-007	-6.319	-6.455
	CaHSO4+	2.999e-007	2.192e-007	-6.523	-6.659
-0.136	Fe_triSO4+	1.583e-008	1.157e-008	-7.801	-7.937
-0.136	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
-0.136					
-0.545	Fe_triHSO4+2	4.013e-013	1.145e-013	-12.397	-12.941
0.041	Fe_dis04	1.196e-023	1.313e-023	-22.922	-22.882
-0.136	Fe_diH904+	4.365e-028	3.190e-028	-27.360	-27.496

-----Saturation indices----

Phase	SI log IA	P log KT	
Halite Hausmannite Manganite O2(g) Pyrochroite Pyrolusite	-8.93 52.1 -1.11 24.2 -0.78 -3.6 -11.57 3.6 3.45 44.8	-8.34 -8.48 -2.86 2 -1.47 4 -17.09 -4.58 -3.15 -1.51 2 -1.00 4 1.58 0 61.03 3 25.34 8 -2.89 3 15.20 3 41.38 7 -11.13	CaCO3 CaCO3 CH4 CO2 CaMg(CO3)2 CaSO4:2H2O H2 H2O H2O H2S NaCI Mn3O4 MnOCH C2 Mn(CH)2 MnCQ

End of simulation.

Reading input data for simulation 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