

UBC Social, Ecological Economic Development Studies (SEEDS) Student Reports

**C.K Choi Greywater Wetland Performance Assessment**

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**An Assessment of the Greywater and Composting  
Toilet Tea Leach Field Geochemistry at the C.K.  
Choi Building, University of British Columbia  
Vancouver Campus**

By

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A Thesis Submitted for the Partial Fulfillment of the  
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## **Abstract**

The geochemistry of a wetland system around the C.K. Choi Building on the University of British Columbia's Vancouver Campus was assessed. The wetland system accepts compost tea from 5 composting toilets in the building as well as greywater from the building sinks. The system was estimated to receive approximately 400L/day and has an area of 30m<sup>2</sup> and a depth of approximately 1m. Dilution and geochemical processes reduce the concentrations of trace metals and nutrients in the inflowing greywater and compost tea. Removal efficiencies of 99% for ammonia were observed in the system and are attributed to nitrification and dilution. Nitrate/nitrite sees removal efficiencies of 98%, due to denitrification and dilution. Manganese(IV) and Iron (III) reduction is observed to produce soluble Mn(II) and Fe(II) which are then easily adsorbed by phosphorus and precipitated as hydroxyapatite, MnHPO<sub>4</sub>, vivianite and strengite. Sulfate reduction also takes place and facilitates the precipitation of metal sulfides such as iron sulfide.

## Table of Contents

1. Introduction.....	5
1.1 Wetlands .....	6
1.2 Geological Surroundings .....	8
2. Fieldwork .....	10
2.1 Materials and Testing Methods.....	11
2.1.1 pH Testing.....	11
2.1.2 Nutrient Testing .....	11
2.1.3 Inductively Coupled Plasma Emission Spectrometry (ICP) Analysis .....	12
2.1.4 Phreeqc Simulation .....	12
3. Background Literature Review .....	13
3.1 Nitrogen Removal.....	13
3.2 Organic Matter Oxidation .....	15
3.3 Plant Uptake.....	17
4. Performance Indicators .....	18
4.1 Chemical Indicators .....	19
4.1.1 Total Nitrogen.....	20
4.1.2 Manganese (IV) Reduction .....	20
4.1.3 Iron(III) Reduction.....	21
4.1.4 Sulphate Reduction .....	21
4.1.5 Phosphorus Removal .....	22
4.1.6 Alkalinity .....	25
4.2 Physical Indicators .....	25
4.2.1 Loading Rate.....	25
5. Results.....	26
6. Analysis.....	28
6.1 Dilution Effects.....	28
6.2 Loading Rate.....	29
6.3 Rate Constant and Mass Balance .....	30
6.4 Removal Efficiencies .....	31
6.5 Phreeqc Simulation .....	32
6.5.1 Assumptions.....	32
6.5.2 Results.....	33
6.5.3 Discussion .....	34
7. Discussion.....	35
7.1 pH.....	35
7.2 Ammonia.....	36
7.3 Nitrate/Nitrite .....	36
7.4 Mn(IV)-Fe(III) Reduction, Sulphate Reduction and Phosphorus Removal .....	36
8. Conclusion .....	37
References.....	39
Appendix A: Lachat QuickChem FIA+ Analysis Methods.....	41
Appendix B: ICP Data .....	43
Appendix C: Phreeqc Simulation Data.....	45

## **List of Figures**

- Figure 1: C.K. Choi Wetland System (Oberlander 2008)
- Figure 2: Plan View of C.K. Choi Wetland System (Oberlander 2008)
- Figure 3: Cross-Sectional View of C.K. Choi Wetland System (Oberlander 2008)
- Figure 4: Map of the UBC Campus (Google Maps)
- Figure 5: Cross Section of Point Grey Cliff Large Scale Stratigraphy (Dakin 2002)
- Figure 6: Model Development for Nitrogen Removal (Sonavane 2009)
- Figure 7: Dilution Test

## **List of Tables**

- Table 1: Liquid Samples
- Table 2: Composition of Septic System Effluent from Ptacek's Study (1998)
- Table 3: Organic Matter Oxidation (Ptacek, 1998)
- Table 4: Phosphorus Removal (Spiterri et al. 2007)
- Table 5: pH Results
- Table 6: Ortho-phosphate Results
- Table 7: Chloride Results
- Table 8: Ammonia Results
- Table 9: Nitrate/Nitrite Results
- Table 10: Concentrations (mg/L) of Trace Metals Retrieved in November 2008
- Table 11: Concentrations (mg/L) of Trace Metals Retrieved in March 2009
- Table 12: Removal Efficiencies
- Table 13: Phreeqc Output Saturation Indices

# 1. Introduction

The C. K. Choi Building which contains the Institute of Asian Research on the University of British Columbia campus was selected to be a demonstration green building in 1992 as part of a half-billion dollar expansion program of the UBC campus. The building has a 3,000m<sup>2</sup> floor space and \$4.5million budget. As part of the initiative, a greywater recycling system and composting toilets were implemented. The building contains 3,000 square meters of office space, workstations and seminar rooms. The building has 5 composting toilets. At the moment, there are approximately 200 people who consistently occupy the building and are regular toilet users.

A component of the building design is a 15 meter long rubble wetland system with an open end that processes the tea from the composting toilets as well as the greywater from the sinks. The compost tea and greywater mixture is discharged by being pumped up to the wetland where it flows a few feet under the ground surface, in a perforated pipe. Vegetation, mainly reeds, throughout the wetland uses the effluent for moisture and nutrients, in the process removing pathogens and harmful compounds. The filtered end product finally leaves the wetland and acts as irrigation in the natural ground.

The purpose of this thesis is to assess the physical and chemical factors that influence the performance of the rubble wetlands of the C. K. Choi Building. The nutrients and trace metals concentrations of the influent and effluent of the wetland is characterized. The wetland geochemistry and physical characteristics will also be compared to other similar wetland systems in environments comparable to Vancouver's.

## 1.1 Wetlands

Wetlands have characteristics of both aquatic and terrestrial systems. They are a transition from one system to the next, characterized by a water table at or near the surface or by a land covered by shallow water. A wetland can function as a chemical sink, retaining more nutrients or sediments than it is releasing. This is due to a variety of properties: wetlands accumulate organics and retain nutrients and sediments; they are autotrophic systems, converting inorganic nutrients to organic biomass; they are calm, low velocity systems and so are good sedimentation basins; and they provide an excellent soil-water contact zone for biochemical processes (Mitsch & Fennessy 1991).

Wetlands are subject to seasonal changes. During the summer, the uptake of chemicals by plants and immobilization of nutrients by flora creates retention of nutrients in the system. When the flora dies, nutrients are left to decompose and leach back into the water stream. In fall and spring, there is a net release of nutrients (Mitsch & Fennessy 1991).

The following image of the C.K. Choi Building's wetland system was taken during the summer months. As can be seen, there are numerous reeds and tall grasses growing on a gravel bed.



Figure 1: C.K. Choi Wetland System (Oberlander 2008)

The next two images are, respectively, a plan and a cross-sectional view of the wetland system around the C.K. Choi Building. The wetland is approximately 15m long, 2m wide and 1m deep. The cross-sectional schematic shows that the wetland receives water from the sinks, the composting toilets and some from the building drains.

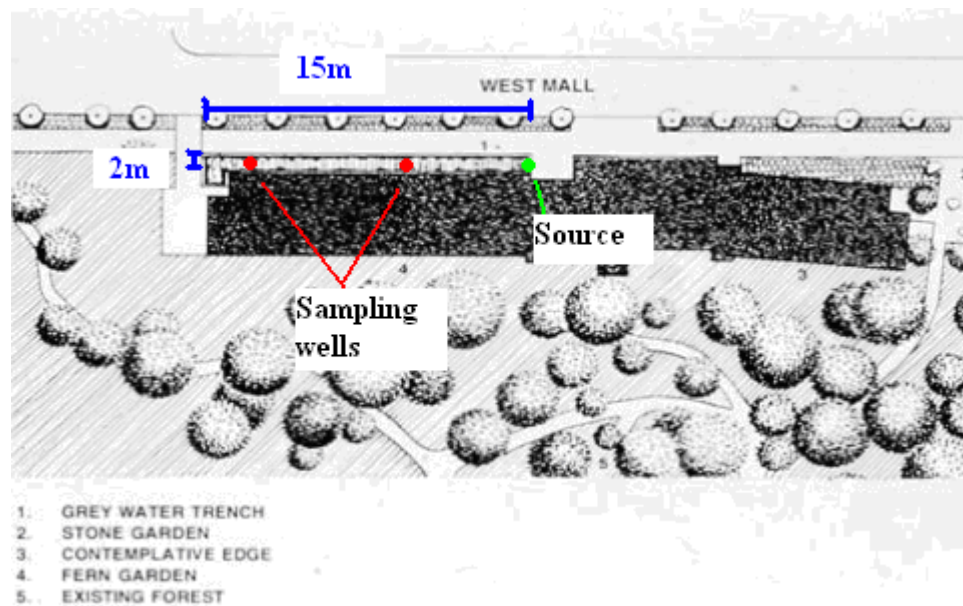


Figure 2: Plan View of C.K. Choi Wetland System (Oberlander 2008)



## GRAY AND STORM WATER DISTRIBUTION SYSTEM

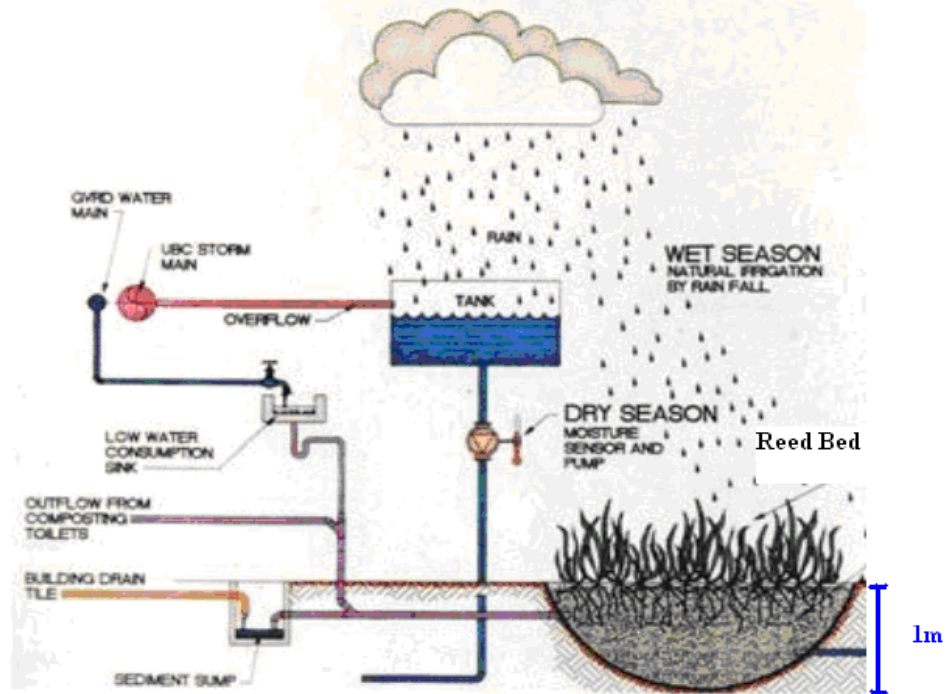


Figure 3: Cross-Sectional View of C.K. Choi Wetland System (Oberlander 2008)

## 1.2 Geological Surroundings

The following image shows the location of the C.K. Choi Building on the UBC campus. The C.K. Choi Building is located on the North-West side of the campus, close to the cliffs leading down to the Strait of Georgia.

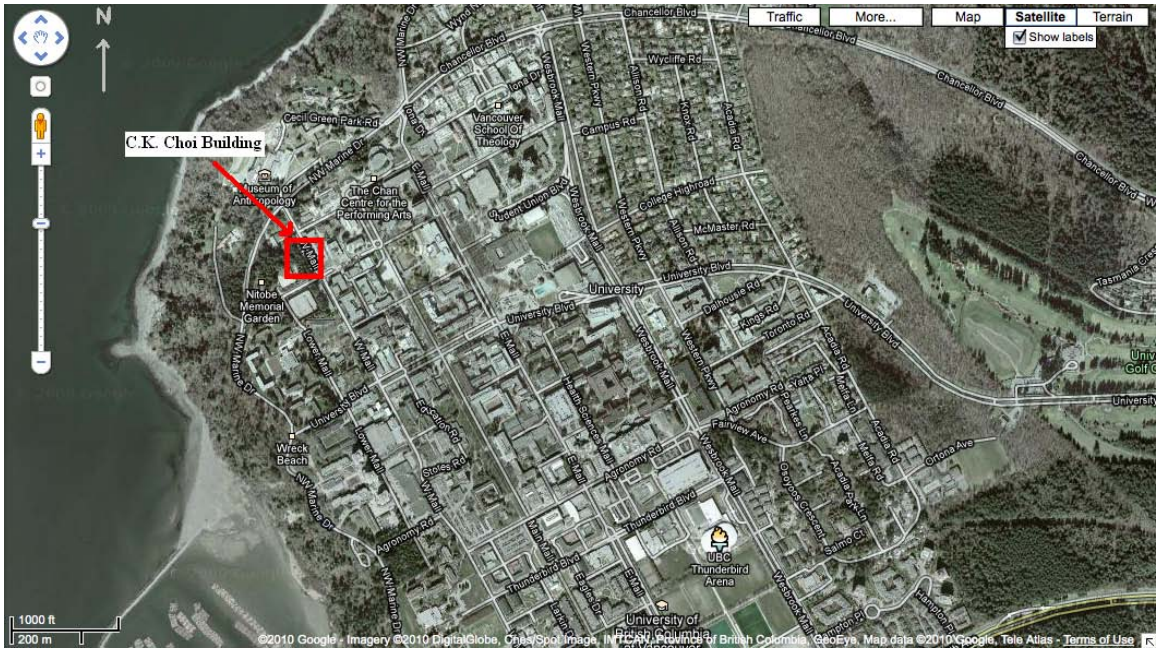


Figure 4: Map of the UBC Campus (Google Maps)

In the West Point Grey/UBC area, the stratigraphy allows for two water tables. There are two aquifers, one at sea level and another approximately 30m above that. The stratigraphy can be determined from observation of the UBC cliffs approximately 100m from the C.K. Choi building. On average, the stratigraphy of the slope consists of a 3m thick layer of glacial till, underlain by about 30m of sand and interbedded silt and clay until the upper aquifer. Under this, there is about 30m of dense silt overlying the second, lower aquifer at beach level. See Figure 5 below for reference:

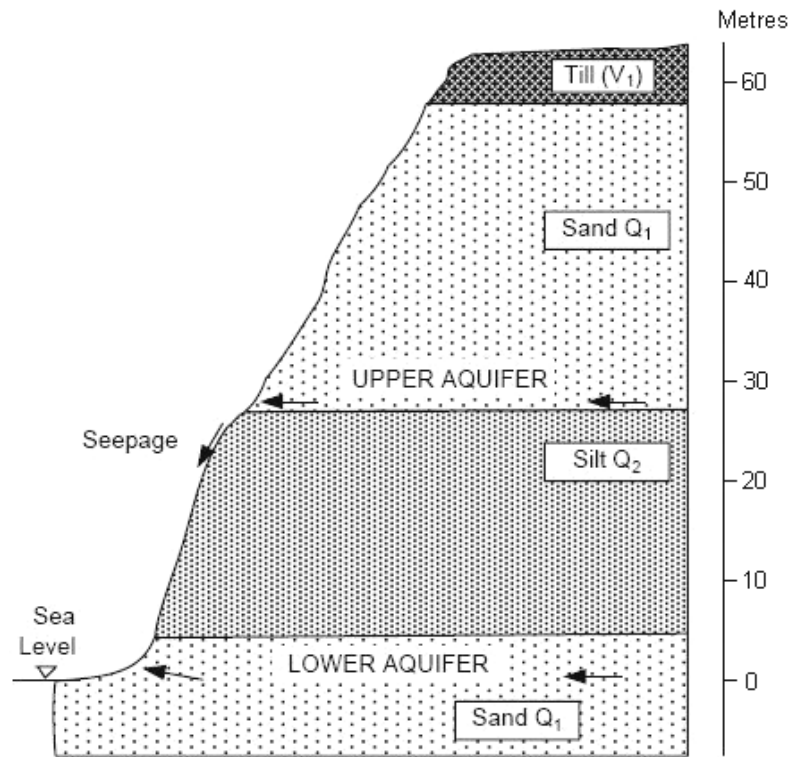


Figure 5: Cross Section of Point Grey Cliff Large Scale Stratigraphy (Dakin 2002)

## 2. Fieldwork

Two distinct rounds of samples were collected and analyzed. Water samples were collected from two different wells along the wetland (see Figure 2), one at the end of the wetland and one in the middle of the wetland closer to where the untreated compost tea and greywater first enter. A third and fourth sample were also taken from the tanks where the tea and greywater are stored inside the building. These liquids are stored in separate tanks where they sit until their level reach a certain height and are then pumped up to the wetland. The following table lists the location of the samples collected, their volumes, methods of preservation and their use:

Table 1: Liquid Samples

Location	Date	Volume (mL)	Method of Preservation	Parameters Measured
Compost Tea Tank	Nov-08	120mL	Air tight seal and refrigerate. Acidified with HCl before using Inductively Coupled Plasma Emission Spectrometer	pH, P, Cl, N-NH <sub>4</sub> , NO <sub>x</sub> , trace metals
Greywater Tank				pH, P, Cl, N-NH <sub>4</sub> , Nox
Borehole Closest to Source				pH, P, Cl, N-NH <sub>4</sub> , NO <sub>x</sub> , trace metals
Borehole Furthest From Source				pH, P, Cl, N-NH <sub>4</sub> , NO <sub>x</sub> , trace metals
Borehole Closest to Source	Mar-09			pH, P, Cl, N-NH <sub>4</sub> , NO <sub>x</sub> , trace metals
Borehole Furthest From Source				pH, P, Cl, N-NH <sub>4</sub> , NO <sub>x</sub> , trace metals

## 2.1 Materials and Testing Methods

Four different analyses were conducted to assess the wetland water: pH probe analysis, nutrient analysis, Inductively Coupled Plasma Emission Spectrometry (ICP) analysis, and phreeqc simulation.

### 2.1.1 pH Testing

To test the pH of the samples, I used a pH probe directly on-site. Firstly, I calibrated the pH probe with standard buffers: pH 4 solution, pH 7 solution and pH 10 solution. Once the system was calibrated, I was able to measure the pH for the samples. I rinsed the pH probe with distilled water after each use to ensure that it was not contaminated.

### 2.1.2 Nutrient Testing

Nutrients, consisting of ammonia, chloride, nitrate/nitrite and orthophosphate were measured in the Soil Water Environment Laboratory at UBC. Samples were run

with blanks so as to detect any potential errors or contamination from sample preparation. The instrument used is called the Lachat QuickChem FIA+ (8000 series) and analyzed the concentrations automatically. A summary of the methods used by this instrument can be found in Appendix A.

### **2.1.3 Inductively Coupled Plasma Emission Spectrometry**

#### **(ICP) Analysis**

The ICP is used to determine cation and trace metal concentrations on samples acidified to  $\text{pH} < 1.5$  with HCl. It works by injecting a nebulized mist from a liquid into the center of an argon plasma. A plasma is created by a flow of gas in a high energy field which ionizes the gas and causes intense heating, up to 10,000 K. As the mist of the sample enters the plasma, the heat dissociates most chemical compounds. The energy that the atoms absorb causes them to undergo excitation and ionization energy transitions. These transitions produce spectral emissions that are characteristic of the elements being excited. The spectrum produced by the plasma is separated into individual spectral lines by the ICP's spectrometer, which the computer can then analyze as concentrations of specified elements (Ammann, 2007).

Element concentrations are given in parts per million (ppm) on a sample volume basis, taking into account dilutions prior to testing.

### **2.1.4 Phreeqc Simulation**

Phreeqc is a software tool for the simulation of one-dimensional unsaturated flow and solute transport. Inverse modeling was used with Phreeqc to follow the chemical changes that occur as the input water evolves along the flow path. Inverse modeling

calculates the moles of minerals and gases that enter or leave the system to account for the changes in composition along the flow path.

### **3. Background Literature Review**

To date, researchers from around North America have conducted analyses on wetlands that process greywater, stormwater and sewage. Experiments have been conducted on sites of different scales, from industrial and commercial size wetlands to domestic wetland systems. Different experiments have emphasized their analysis on different characteristics of wetlands or different processes that occur in them, ranging from nitrogen removal to organic matter oxidation to plant uptake of nutrients. Their findings are summarized below.

#### **3.1 Nitrogen Removal**

Tuncsiper (2009) conducted a study to determine appropriate conditions for nitrogen removal. He looked at hydraulic loading rates, nitrogen loading rates, effluent recirculation, plant uptake and seasonal change on nitrogen removal efficiency.

Tuncsiper states that the most important processes that remove nitrogen from domestic sewage in small constructed wetlands are nitrification and denitrification (see Equation 2 and Table 3 respectively for equations). He quotes a study by Platzer (1997) that showed that for a constructed wetland with 250 to 630 g N/m<sup>2</sup>/yr loading rates, the removal efficiency of total nitrogen ranges from 40% to 55%. This study also showed that horizontal constructed wetlands have a high denitrification capacity and vertical constructed wetlands have a high nitrification capacity. So by combining these two flows, higher total nitrogen removal efficiencies are optimized.

Tunciper's study found that the raw wastewater had a pH of 7, total nitrogen of 52.9mg/L, ammonium ( $\text{NH}_4^+(\text{aq})$ ) of 36.8mg/L and nitrate ( $\text{NO}_3^-$ ) of 2.32mg/L. Nitrite ( $\text{NO}_2^-$ ) concentrations were below 0.3mg/L. His study showed that the aerobic conditions in the vertical constructed wetland led to high nitrification rates and the anaerobic conditions in the horizontal constructed wetland led to high denitrification rates. Also, during colder months, the removal efficiencies decreased because the temperature dropped from 23 to 9 degrees Celcius.

The temperature dependent rate constant ( $K_T$ ) for ammonium and nitrate were calculated by Tuncsiper using the following equation:

$$\ln\left(\frac{C_e - C^*}{C_i - C^*}\right) = -K_T \bullet t \quad (\text{Equation 1})$$

Where  $C_e$  is the final concentration,  $C_i$  is the initial concentration,  $C^*$  is the irreducible background concentration and  $t$  is the hydraulic residence time.

Tuncsiper quotes studies by Bavor et al (1988), Reed & Brown (1995) that calculate nitrification rate constants of 0.107L/d, 0.4107L/d respectively. He also quotes a study by Reddy & Patrick that calculates denitrification rate constants of 0.004 to 2.57L/d.

These study conditions are similar to those of the C.K. Choi wetlands in its pH conditions. However, they are dissimilar in that the nitrate/nitrite and ammonium concentrations are approximately ten times the ones found in C.K. Choi wetlands, which is expected since the C.K. Choi building does not produce as much sewage as was observed in Tuncsiper's study and its loading rate is smaller. Also, the summer and winter temperatures around UBC usually range between 11 and -5 degrees Celcius, lower than those measured for this study.

### 3.2 Organic Matter Oxidation

Ptacek (1998) studied the major ion and trace metal geochemistry of a septic plume in a shallow sand aquifer, much like the one around the C.K. Choi building. She studied the geochemical processes linked with the movement and exchange of nutrients with their host environment along their flow path.

Septic system effluent shows high levels of dissolved organic carbon, ammonia, phosphorus, and pathogens. The study by Ptacek looks at an area contaminated with blackwater (wastewater from toilets and showers). The water use in the area reaches 2500L/day and is gravity-fed from a holding tank to a tile bed. This loading rate and consequently the nutrient concentrations in the effluent are considerably higher than those observed in the wetland around the C.K. Choi building. Concentrations in the holding tank were as follows:

Table 2: Composition of Septic System Effluent from Ptacek's Study (1998)

<b>Parameter</b>	<b>Concentration (mg/L)</b>
DOC	31.8
NH <sub>4</sub>	97.9
Total P	11.8
Ca	83.6
Mg	12.9
Na	42.8
K	20.6
Cl	57.0
SO <sub>4</sub>	34.1
SiO <sub>2</sub>	9.65
Fe	0.599
Mn	0.480
Cu	0.029
Zn	0.069
Al	0.10



In her study Ptacek observed the highest concentrations of dissolved organic carbon (DOC) near to the septic plume source, decreasing with distance from the bed. Removal efficiencies ranged from 60 to 80%.

The main oxidant of ammonia is oxygen. O<sub>2</sub> has low solubility and as a result, most oxidation takes place in the unsaturated zone. Oxidation is not, however, excluded from the saturated zone; it only occurs at much slower rates and occurs when oxidation is incomplete in the unsaturated zone. NH<sub>4</sub><sup>+</sup>(aq) was found in the saturated zone, which means that oxidation in the unsaturated zone is incomplete. This could have several causes: short residence times in the unsaturated zone due to high permeability of the sands, high loading rates, and a shallow water table; or insufficient active microbes due to the sporadic discharge of wastewater.

PO<sub>4</sub> removal efficiencies were approximately 80%, which agrees with other sites' removal efficiencies of 50 to 80%. The main removal mechanism is through precipitation as hydroxyapatite and ferrihydrite.

Decreases in pH were observed and agree with the expected changes due to the release of CO<sub>2</sub> from organic matter oxidation and of H<sup>+</sup> from NH<sub>4</sub><sup>+</sup>(aq) oxidation (see following equation):



The study site contained excess carbonate minerals. The decrease in pH due to CO<sub>2</sub> release from organic matter oxidation and H<sup>+</sup> release is expected to lead to carbonate mineral dissolution, which results in an increase in alkalinity, Ca<sup>2+</sup> concentrations, and other cations from the carbonate minerals. Alkalinity values ranged from 200mg/L at the effluent plume margins and 350-500mg/L in the plume core.

In Ptacek's study site, high concentrations of Mn and Fe were observed near the leachate plume, likely due to reductive dissolution of Mn(IV) oxides coupled with DOC oxidation and due to reductive dissolution of Fe(III) oxyhydroxide solids coupled with DOC oxidation respectively. Furthermore, the upper meters of sand are stained with an orange colour, indicating the presence of Fe(III) oxyhydroxide solids.

N/Cl ratios are assumed to remain relatively constant over time in the raw effluent. In Ptacek's study, given that the N/Cl ratio decreased over time, it was assumed that there was loss of N during transport from the source area. The loss of total N could be due to nitrate reduction, dilution, oxidation of  $\text{NH}_4^+(\text{aq})$ , or cation exchange reactions with  $\text{NH}_4^+(\text{aq})$ .

### **3.3 Plant Uptake**

The performance of wetlands depends on numerous factors: influent characteristics, loading rate, storage capacity, the design of the wetland system, and environmental factors such as light and temperature. To better understand the components and mechanisms that determine the level of performance of a wetland system, Breen (1990) conducted a study using a mass balance approach to investigate individual aspects of the system. The approach intended to "describe system performance, indicate the relative size and importance of various components, suggest which removal processes are operating, and allow quantification of the removal rates" (Breen 1990).

The study wetland system consisted of washed gravel as substratum and rhizomes of *Typha Orientalis* planted in the gravel. The system had an upflow format, with influent entering at the bottom and effluent collected at the top of the system, much like the one

around the C.K. Choi building. Results showed that the planted system removed over 80% of the chemical oxygen demand(COD), a measure of the organic compounds in the water, and 95% of the N and P. In the unplanted system, however, there as little as 7% N storage, demonstrating the plant uptake has a large effect on N absorption. Using the mass balance approach, Breen concluded that there are only two mechanisms that remove P from the system: adsorption onto the substratum and absorption by plants. Gravel has a low adsorption capacity and so adsorption did not prove useful for nutrient removal in this experiment. Plants were the major nutrient sink for N and P, absorbing 50% of the influent N and 67% of the influent P. In addition to this, denitrification was also determined to be a significant process for N removal, in both the planted and unplanted systems (Breen 1990).

#### **4. Performance Indicators**

In this analysis, I am observing a passive treatment system. Passive treatment is identified as “the deliberate improvement of water quality using only naturally-available energy sources (eg. gravity, microbial metabolic energy, photosynthesis) in systems which require only infrequent (albeit regular) maintenance in order to operate effectively over the entire system design life” (Younger et al. 2002). Therefore, I will not be looking at inputs of artificial energy or chemical reagents. With an understanding of the literature, chemistry and related experiments, the chemical and physical processes that are expected to occur in the C.K. Choi wetlands can be identified.

## 4.1 Chemical Indicators

With the migration of the compost tea and greywater, N and P are released from organic compounds and oxidation of DOC leads to higher concentrations of  $\text{NO}_3^-$ ,  $\text{PO}_4$ ,  $\text{CO}_2$  and  $\text{H}^+$ . The principal oxidant of DOC and ammonia is oxygen. Most oxidation of the effluent takes place in the unsaturated zone. However, oxidation can occur in the saturated zone, only at much slower rates; this occurs when oxidation is incomplete in the unsaturated zone. Therefore, if products of organic matter oxidation reactions are found in the saturated zone, it is an indicator that oxidation is incomplete in the unsaturated zone. The following table lists the main oxidation reactions that take place in the effluent and their free energy. A more negative free energy means that the reaction is more likely to occur.

Table 3: Organic Matter Oxidation (Ptacek, 1998)

Process	Reaction <sup>a</sup>	Free energy <sup>b</sup> (kcal mol <sup>-1</sup> )
O <sub>2</sub> reduction	$\text{CH}_2\text{O} + 1/2 \text{O}_2 = \text{HCO}_3^- + \text{H}^+$	- 118.8
Denitrification	$\text{CH}_2\text{O} + 4/5 \text{NO}_3^- = 2/5 \text{N}_2(\text{g}) + \text{HCO}_3^- + 1/5 \text{H}^+ + 2/5 \text{H}_2\text{O}$	- 112.7
Manganese(IV) reduction	$\text{CH}_2\text{O} + 2\text{MnO}_2(\text{s}) + 3\text{H}^+ = 2\text{Mn}^{2+} + \text{HCO}_3^- + 2\text{H}_2\text{O}$	- 84.9
Iron(III) reduction	$\text{CH}_2\text{O} + 4\text{Fe}(\text{OH})_3(\text{s}) + 7\text{H}^+ = 4\text{Fe}^{2+} + \text{HCO}_3^- + 10\text{H}_2\text{O}$	- 26.8
Sulphate reduction	$\text{CH}_2\text{O} + 1/2 \text{SO}_4^{2-} = 1/2 \text{HS}^- + \text{HCO}_3^- + 1/2 \text{H}^+$	- 23.9
Methane fermentation	$\text{CH}_2\text{O} + 1/2 \text{H}_2\text{O} = 1/2 \text{CH}_4 + 1/2 \text{HCO}_3^- + 1/2 \text{H}^+$	- 21.6

<sup>a</sup>Reactions from Freeze and Cherry (1979).

<sup>b</sup>Free energy data from Garrels and Christ (1965) and Brock et al. (1984); calculated for pH = 7.0

In the saturated zone, oxygen is not present in high enough concentrations to completely oxidize DOC and  $\text{NH}_4^+(\text{aq})$ ; their oxidation depends on another electron acceptor. The expected sequence of reactions goes from denitrification, to reductive dissolution of Mn-oxides, followed by reductive dissolution of Fe-oxides (see Table 3 above). These processes are indicated by a decrease in  $\text{NO}_3^-$  concentrations and an increase in dissolved  $\text{Mn}^{2+}$  and  $\text{Fe}^{2+}$  concentrations. Other reactions, only under strongly

reducing conditions, include sulfate reduction and methanogenesis (see Table 3 above) (Ptacek 1998).

### 4.1.1 Total Nitrogen

The following processes were used in the model development for nitrogen removal:

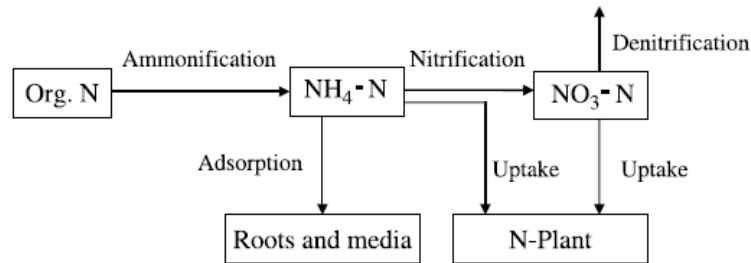


Figure 6: Model Development for Nitrogen Removal (Sonavane 2009)

Ammonification, which occurs in the composting tanks, transforms the organic nitrogen into  $NH_4N$  and nitrification transforms  $NH_4N$  into nitrates ( $NO_3^-$ ). Overall the nitrogen concentration increases with nitrification and decreases with denitrification.

$NH_4^+(aq)$  is released by aerobic degradation. It is then removed from solution by nitrification and adsorption. The process of nitrification produces nitrate ( $NO_3^-$ ) (see Equation 2 on page 15), also increasing the  $H^+$  concentration, thus decreasing the pH of the solution. So, drops in dissolved  $NH_4^+$  concentrations are due to either dilution or due to oxidation or cation exchange reactions (Ptacek 1998). Denitrification can then occur (see Table 3 on page 18). This process uses  $NO_3^-$  to produce gaseous nitrogen ( $N_2(g)$ ).

### 4.1.2 Manganese (IV) Reduction

Reducing conditions, as are present in the wetland system around the C.K. Choi Building, reduce manganese to its reduced state of  $Mn^{2+}$ . The reductive dissolution of

Mn-oxyhydroxides is marked by an increase in pH and DOC. Mn(IV) is more readily reduced with organic compounds than Fe(III) and so reduction of Mn(IV) occurs before that of Fe(III). In some instances, Mn(IV) and Fe(III) reduction can occur simultaneously. This is the case with unstable Fe minerals and organically complexed Fe<sup>3+</sup>. In most cases however, such as under near neutral pH conditions, organic compounds such as oxalate, pyruvate and syringic acid reduce Mn(IV) before Fe(III) is reduced (Grybos et al. 2009).

#### **4.1.3 Iron(III) Reduction**

Redox indicators include the redox couples NH<sub>4</sub><sup>+</sup> - NO<sub>3</sub><sup>-</sup> and Mn<sup>4+</sup> - Mn<sup>2+</sup>, as mentioned above, and Fe<sup>2+</sup> - Fe<sup>3+</sup>. Reducing conditions cause iron to be in the ferrous oxidation state (Fe<sup>2+</sup>). Between a pH of 5 to 9, Fe<sup>3+</sup> concentrations are low due to the solubility of ferric oxyhydroxide minerals such as ferrihydrite (Fe(OH)<sub>3</sub>), producing Fe<sup>2+</sup> (see equation in Table 3). The presence of more than 0.1 mg/L Fe is a good indicator of reducing conditions.

#### **4.1.4 Sulphate Reduction**

Reduction of sulphate improves water quality in several ways. Firstly, sulphate reduction increases alkalinity and pH. Secondly, the reduction of sulfate to sulfide induces the precipitation of metal-sulfide minerals that have low solubility. Thirdly, sulfate reduction promotes the formation of gaseous sulfur species that diffuse into the atmosphere. In Table 3, we can see how sulfate is reduced to produce sulfide (H<sub>2</sub>S) in a reducing environment such as the wetland observed. At pH values higher than 4.5, sulfate

reduction also produces bicarbonate. If Fe or other metals are present, they can combine with sulfide as is demonstrated in equation 3.



If the sulfide gas does not react with a metal, it can diffuse upwards and escape into the atmosphere.

According to a study by Wilderman et al. (1990), sulfate reduction and precipitation of metal sulfides removes 95% of dissolved Fe, Zn, Mn, Ni and Cd.

#### 4.1.5 Phosphorus Removal

Phosphorus concentrations (~5 – 20 mg/L) normally found in sewage effluent are much higher than the concentrations (~0.30 mg/L) observed in other aquatic environments. Phosphate is absorbed strongly by most sediments and combines with various metal cations such as iron, aluminum, manganese and calcium to form various minerals.

The main processes affecting phosphorus transport are adsorption/desorption and precipitation/dissolution. Phosphate ( $PO_4^{3-}$ ) can be adsorbed by various minerals. It is a proteolytic acid with a negative 3 charge that can protonate to form  $HPO_4^{2-}$ ,  $H_2PO_4^-$  and  $H_3PO_4$ . Under near neutral groundwater pH conditions,  $HPO_4^{2-}$  and  $H_2PO_4^-$  are the two dominant forms present. Therefore, if positively charged minerals are present such as Al, Mn(IV) and Fe(III) containing oxides and oxyhydroxides, these anions will be adsorbed (See Table 4 below).

As for precipitation and dissolution of  $PO_4$  containing solids, the most common solids containing  $PO_4$  are Al, Fe and Ca solids (Nriagu and Dell, 1974). At low

temperatures, the solids that control the dissolution of  $PO_4$  include hydroxyapatite ( $Ca_5(PO_4)_3OH$ ), variscite ( $AlPO_4 \cdot 2H_2O$ ), strengite ( $FePO_4 \cdot 2H_2O$ ), and vivianite ( $Fe^{2+}_3(PO_4)_2 \cdot 8H_2O$ ) (Strumm and Morgan 1981). Groundwater that contains phosphate and carbonate minerals is usually saturated with respect to hydroxyapatite, but its formation is kinetically limited. Also, when both phosphate and  $CaCO_3$  are present, precipitation of  $Ca PO_4$  is likely to occur. Siderite ( $FeCO_3$ ) can also be a controlling factor for the concentration of dissolved  $PO_4$ , by keeping ferrous iron concentrations low (Ptacek 1998, Akratos 2009). The portion not sorbed to sediments is available for phytoplanktons to uptake or it just flows out through the water stream.



Table 4: Phosphorus Removal (Spiterri et al. 2007)

C. Spiterri et al. / Journal of Contaminant Hydrology 92 (2007) 87–108

Slow P adsorption/desorption into Fe oxides *	$\Sigma\text{PO}_4(\text{aq}) + \text{Fe}(\text{OH})_3 \leftrightarrow \text{P}_{\text{s-slow}}$	$\text{Rate} = -k_{\text{Fe}}(0.4^x[\text{Fe}(\text{OH})_3] - [\text{P}_{\text{s-slow}}])([\Sigma\text{PO}_4(\text{aq})] - [\Sigma\text{PO}_4(\text{eq})])$
Slow adsorption/ desorption into calcite **	$\Sigma\text{PO}_4(\text{aq}) + \text{CaCO}_3 \leftrightarrow \text{P}_{\text{s-slow}}$	$\text{Rate} = -k_{\text{Fe}}(0.55^y[\text{CaCO}_3] - [\text{P}_{\text{s-slow}}])([\Sigma\text{PO}_4(\text{aq})] - [\Sigma\text{PO}_4(\text{eq})])$
<i>Acid/base equilibria and equilibrium sorption</i>		
Carbonate dissociation	$\text{CO}_2 + \text{H}_2\text{O} \leftrightarrow \text{H}^+ + \text{HCO}_3^-$	$K_{\text{eq1}} = \frac{[\text{H}^+][\text{HCO}_3^-]}{[\text{CO}_2]}$
Carbonate dissociation	$\text{HCO}_3^- \leftrightarrow \text{H}^+ + \text{CO}_3^{2-}$	$K_{\text{eq2}} = \frac{[\text{H}^+][\text{CO}_3^{2-}]}{[\text{HCO}_3^-]}$
Phosphate dissociation	$\text{H}_2\text{PO}_4^- \leftrightarrow \text{H}^+ + \text{HPO}_4^{2-}$	$K_{\text{phos1}} = \frac{[\text{H}^+][\text{HPO}_4^{2-}]}{[\text{H}_2\text{PO}_4^-]}$
Phosphate dissociation	$\text{HPO}_4^{2-} \leftrightarrow \text{H}^+ + \text{PO}_4^{3-}$	$K_{\text{phos2}} = \frac{[\text{H}^+][\text{PO}_4^{3-}]}{[\text{HPO}_4^{2-}]}$
Ammonium sorption	$\text{NH}_4^+ \leftrightarrow \text{NH}_4(\text{ads})$	$K_{\text{N}}\phi = \frac{[\text{NH}_4(\text{ads})]}{[\text{NH}_4^+]}$
Fast P adsorption/desorption on Fe oxide *	$\Sigma\text{PO}_4(\text{aq}) \leftrightarrow \text{P}_{\text{s-fast}}$	$[P_{\text{s-fast}}] = \frac{K_f 0.1^x [\text{Fe}(\text{OH})_3] [\Sigma\text{PO}_4(\text{aq})]}{1 + K_f [\Sigma\text{PO}_4(\text{aq})]}$
Fast P adsorption/desorption on calcite **	$\Sigma\text{PO}_4(\text{aq}) \leftrightarrow \text{P}_{\text{s-fast}}$	$[P_{\text{s-fast}}] = \frac{K_f 0.05^y [\text{CaCO}_3] [\Sigma\text{PO}_4(\text{aq})]}{1 + K_f [\Sigma\text{PO}_4(\text{aq})]}$

Parameter values are listed in Table 2.

\* and \*\* Reactions NOT included in simulations of Cambridge case study (1) and Muskoka case study (2), respectively.

<sup>a</sup>CH<sub>2</sub>O represented with an elemental composition (CH<sub>2</sub>O)(NH<sub>3</sub>)<sub>x</sub>(H<sub>3</sub>PO<sub>4</sub>)<sub>z</sub>, where x=150, y=16, z=1; Carbon is assumed to be present as DOC<sub>1</sub> and DOC<sub>2</sub>.

<sup>b</sup>Q=ion activity product/solubility product; If Q>1 → mineral precipitation; If Q<1 → mineral dissolution; h=heavy side operator to switch from precipitation to dissolution and vice versa.

<sup>c</sup>Assuming a P:Fe ratio of 0.5 (Gunnars et al., 2002) and 10% of Fe(OH)<sub>3</sub> is available for fast sorption (Slomp et al., 1996); <sup>d</sup>Assuming a P:Ca ratio of 0.6 (Freeman and Rowell, 1981) and 5% of CaCO<sub>3</sub> is available for fast sorption (Cole et al., 1953).

### **4.1.6 Alkalinity**

Passive treatment systems, or reducing conditions, add alkalinity to wastewater. The wetland contains alkalinity producing materials such as dead plant matter (Walton-Day 2003). A study by Lorah et al (2008) observed alkalinity values of 0.5 to 1meq/L for a naturally attenuating landfill leachate. The study also showed that this value doubled during the wet season when plant growth was higher. Similar results for alkalinity (0.9 to 1.2meq/L) were observed in a natural pond setting in a study by Espinar and Serrano (2008).

## **4.2 Physical Indicators**

### **4.2.1 Loading Rate**

Estimated loading rates at the entrance of the wetland system and retention times were calculated. The total amount of water flowing into the wetland (Q), divided by the area of the study wetland (A), gives an estimate of the loading rate of a wetland (L).

$$L = Q/A \quad \text{(Equation 3)}$$

The turnover rate ( $t^{-1}$ ) is calculated by dividing the loading rate by the average depth of the wetland (d).

$$t^{-1} = L/d \quad \text{(Equation 4)}$$

The retention time (t) is the reciprocal of the turnover rate.

The longer the retention time of the wetland, the longer the water is in contact with the biologically active soil and the greater the rate of physical processes and sedimentation.

## 5. Results

The following tables summarize the lab results obtained for pH and for the concentrations of ortho-phosphate, chloride, nitrate/nitrite, and ammonia in the wetland around the C.K. Choi building. These results were given from the Lachat QuickChem FIA+ (8000 series) instrument.

Table 5: pH Results

Sample ID	pH (Nov 2008)	pH (Mar 2009)
Compost Tea	7.71	
Greywater	4.72	
Effluent closest to source	6.15	7.03
Effluent furthest from source	6.04	6.92

Table 6: Ortho-phosphate Results

Sample ID	Ortho-phosphate (mg P/L) (Nov 2008)
Compost Tea	145.43
Greywater	0.58
Effluent closest to source	6.42
Effluent furthest from source	5.88

Table 7: Chloride Results

Sample ID	Chloride (mg Cl/L) (Nov 2008)
Compost Tea	3017
Greywater	36
Effluent closest to source	66
Effluent furthest from source	79

Table 8: Ammonia Results

Sample ID	Ammonia (mg N-NH <sub>4</sub> /L) (Nov 2008)
Compost Tea	692.9
Greywater	7.8
Effluent closest to source	2.6
Effluent furthest from source	5.4

Table 9: Nitrate/Nitrite Results

Sample ID	Nitrate/Nitrite (mg NO <sub>x</sub> /L) (Nov 2008)
Compost Tea	307.74
Greywater	0.12
Effluent closest to source	3.45
Effluent furthest from source	3.3

The following tables summarize the ICP results for the compost tea and liquid flowing through the C.K. Choi wetlands. The same trace metal was sometimes identified with different wavelengths, so if two different concentrations were identified, the most reasonable concentration was taken. Detection limits were set as follow: 0.1 to 100ppm for P, 10 to 500ppm for S, and 0.1 to 100ppm for all other trace metals. Therefore, if metals were present at lower concentrations than these, they should not be detected by the ICP machine. However, some of the metals were detected at lower concentrations than the standards. I chose to accept this data if concentrations for a particular metal were similar at different wavelengths. The greywater liquid was too thick to run through the ICP machine, so was not analyzed using this instrument.

Table 10: Concentrations (mg/L) of Trace Metals Retrieved in November 2008

<b>Element</b>	<b>Compost Tea</b>	<b>Effluent Closest to Source</b>	<b>Effluent Further From Source</b>
K	6067	27.9	33.81
Na	5910	38.85	38.57
S	1133	5.922	3.546
P	762.7	4.968	5.707
Ca	156.3	6.026	7.592
Fe	9.961	0.325	0.166
Mn	2.014	0.424	0.452
Zn	0.7415	0.3817	1.224
Mo	0.5117	0.02195	0.0155
Cu	0.4639	0.04734	0.1721
Ni	0.06526	0.1603	0.4537

Table 11: Concentrations (mg/L) of Trace Metals Retrieved in March 2009

<b>Element</b>	<b>Effluent Closest to Source</b>	<b>Effluent Further From Source</b>
Na	81.74	94.58
K	42.67	50.56
Ca	16.42	23.04
S	5.37	4.94
P	4.008	5.771
Mg	1.858	3.588
Mn	0.441	0.468
Zn	0.2287	0.218
Fe	0.211	1.025
Ni	0.1141	0.1246
Cu	0.06712	0.01969
Mo	0.01582	0.02117

## 6. Analysis

### 6.1 Dilution Effects

A graph of nutrient concentrations divided by chloride concentration was made to observe how much of the loss of nutrients was due to dilution and how much was due to the geochemical processes occurring in the wetland.

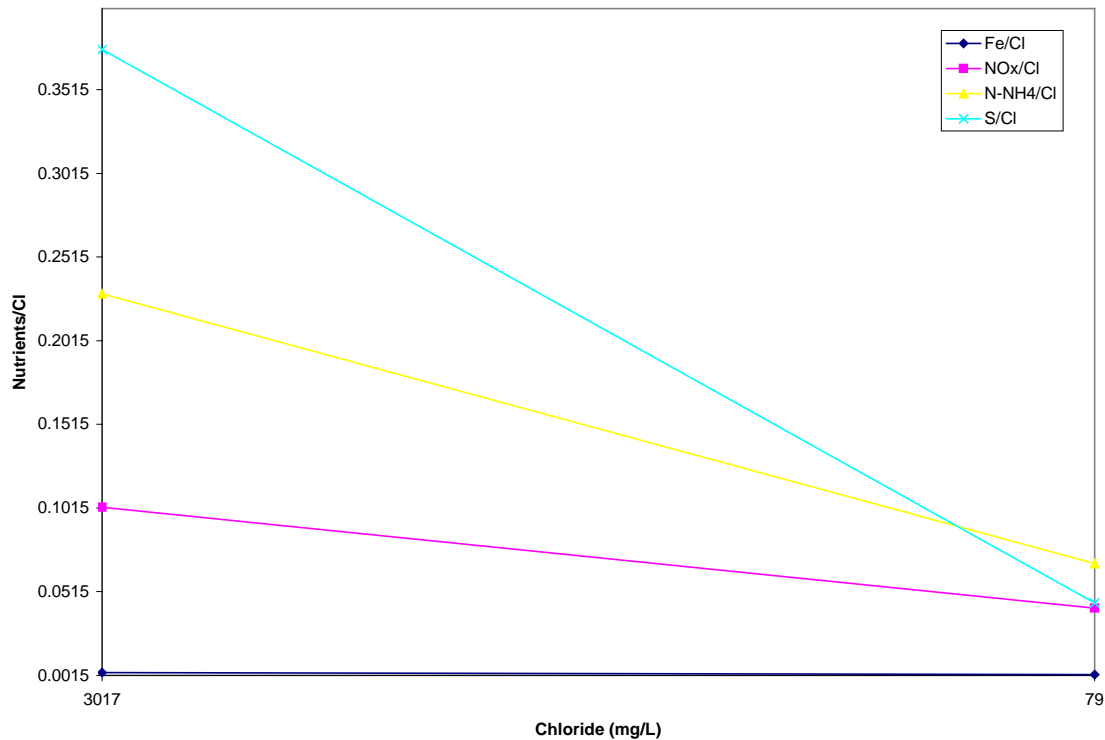


Figure 7: Dilution Test

As is observed from Figure 7 above, the lines for nutrient/Cl over Cl have a negative slope. This means that in addition to dilution, many processes are happening to reduce the concentrations of the nutrients present in the wastewater as it flows through the wetland. These processes will be discussed in Section 7: Discussion.

## 6.2 Loading Rate

A loading rate can be estimated for the wetland system, using equations 3 and 4 (on page 24). In order to remain conservative, I assumed 200 people use the toilets and sinks in the C.K. Choi building. Not everyone will use these washrooms all day, so I assume each person produces 2L of greywater and compost tea per day. This totals as 400L of wastewater per day going into the wetlands. The area of the wetland was assumed to be 20m<sup>2</sup>, giving the wetland a loading rate of 0.02m/day. This loading rate is

smaller than the studies observed in literature (Platzer 1997, Ptacek 1998); however it is a reasonable estimate since not many people occupy this building at this time and so the wetland does not need to support as much wastewater.

Assuming a conservative depth of 0.5m for the wetland, by taking the loading rate divided by the depth of the wetland, a hydraulic residence time can be calculated as 25 days. From the geochemistry changes observed as the wastewater flows through the system, we can confirm that 25 days residence time is sufficient to clean the effluent. From the lab results, we see that significant removal occurs early in the flow system, at the sampling well closest to the source (see Figure 2).

### 6.3 Rate Constant and Mass Balance

As was earlier discussed in Tuncsiper's literature review, the rate constant can be calculated using equation 1. Because of dilution, the calculated rate constants are approximate. Assuming a hydraulic residence time of 25 days and an estimated irreducible background concentration of 3mg/L for nitrate/nitrite, the rate constant for nitrification is calculated as 0.28L/d. This value is comparable to those calculated by Bavor et al (1988) and by Reed & Brown (1995) whose studies showed nitrification rate constants of 0.107L/d, 0.4107L/d respectively.

A mass balance can also be calculated. It was assumed that the compost tea flow is an eighth of the total flow, or 50L/day, and the greywater flow is seven eighths of the total flow, or 350L/day. These flows are estimates. A mass balance for nitrogen can be calculated using equation 5:

$$[NO_x] = \frac{Q_{compost} [NO_x] + Q_{greywater} [NO_x]}{Q_{compost} + Q_{greywater}} \quad (\text{Equation 5})$$

The brackets indicate concentrations. This equation gives a nitrate/nitrite concentration of 38.57mg/L, which is much higher than the 3.45mg/L of nitrate/nitrite observed at the sampling well closest to the source. This is an indication of both dilution and denitrification.

## 6.4 Removal Efficiencies

Removal efficiencies can be calculated using the load. I assumed that the flow through the system did not remain at 400L/day throughout the entire wetland system. I estimated that there was approximately 20L/d of flow lost to infiltration into the gravel. By using the following equation, removal efficiencies for various metals were calculated:

$$1 - \frac{C_2 Q_2}{C_1 Q_1} \cdot 100\% \quad \text{(Equation 6)}$$

Where  $C_2$  is the concentration of the trace metal at the furthest sampling point in the wetland and  $Q_2$  is the flow at the same place,  $C_1$  is the concentration of the trace metal in the compost tea and  $Q_1$  is the flow at the inlet to the wetland.

As mentioned earlier, the flow at the inlet to the wetland is estimated as 400L/day and the flow at the furthest point in the wetland is 380L/day. The following table lists the removal efficiencies for various trace metals.

Table 12: Removal Efficiencies

	<b>P</b>	<b>Nitrate/Nitrite</b>	<b>Ammonia</b>
<b>C2 (mg/L)</b>	5.707	3.3	5.4
<b>Q2 (L/day)</b>	400	400	400
<b>C1 (mg/L)</b>	762.7	307.74	692.9
<b>Q1 (L/day)</b>	380	380	380
<b>Removal Efficiency (%)</b>	99.1	98.8	99.1

These removal efficiencies are high compared to the 80% and 70% removal efficiencies observed for P and N in Tuncsiper (2009) and Ptacek's (1998) studies, but



are closer to the 95% P and N removal efficiencies observed by Breen (1990). The high removal efficiencies observed in the wetland system around the C.K. Choi building are likely due to the concentrations of trace metals and nutrients being low when they enter the system and so are easily removed. Also, as observed by Breen (1990) and Walton-Day (2003), plant uptake is a significant contribution to metal removal. Plants immobilize metals and accumulate them in their structures, a process that takes place in the C.K. Choi wetland system.

## **6.5 Phreeqc Simulation**

The Phreeqc simulation was only run with the compost tea because trace metal data was available not available for the greywater since the ICP machine could not handle the amount of sediment in the greywater. A solution simulating the trace metal concentrations in the compost tea was run through an environment simulating the wetland system. Precipitates were then observed.

### **6.5.1 Assumptions**

Assumptions were necessary while performing the Phreeqc simulation. Firstly, a total sulfur concentration was obtained from the ICP machine. Because an input of either sulfate or sulfide is necessary in Phreeqc, it was assumed that all the sulfur in the compost tea was in its oxidized form as sulfate. This is an appropriate assumption since the wetlands are a reducing environment and sulfate is also observed in wetland studies such as Ptacek's (1998). High sulfide, instead of sulfate, is extremely toxic and is only present in highly alkaline solutions, which is not likely the case for this wetland. Additionally, the nitrate/nitrite concentration obtained from the Lachat QuickChem

analysis was input in the Phreeqc model as nitrate because this is the most likely species present. The model was initially run without a charge balance. The output then gave a positive imbalance to the solution. Cl was then used as a charge balance to give an electrically neutral solution. The electrically balance system allows Phreeqc to run as many processes as it can with the input given.

The input and output Phreeqc files can be found in Appendix C.

### **6.5.2 Results**

The Phreeqc model was used to observe what reactions occurred to produce precipitate from the wastewater running through the wetland system. Looking at the output file, the minerals with positive saturation indices will precipitate out of solution. Table 13 below summarizes the minerals with positive saturation indices.

Table 13: Phreeqc Output Saturation Indices

Mineral	Saturation Index
Chalcopyrite CuFeS <sub>2</sub>	14.5
Pyrite FeS <sub>2</sub>	11.8
Chalcocite Cu <sub>2</sub> S	9.01
Anilite Cu <sub>0.25</sub> Cu <sub>1.5</sub> S	6.43
Djurleite Cu <sub>0.066</sub> Cu <sub>1.868</sub> S	8.88
Blaubleill Cu <sub>0.6</sub> Cu <sub>0.8</sub> S	6.85
Blaubleil Cu <sub>0.9</sub> Cu <sub>0.2</sub> S	6.33
Covellite CuS	5.3
MnHPO <sub>4</sub>	4.78
Greigite Fe <sub>3</sub> S <sub>4</sub>	4.72
Millerite NiS	3.37
Sphalerite ZnS	1.91
N <sub>2</sub> (g)	1.79
Mackinawite FeS	0.85
FeS(ppt)	0.12
Hydroxyapatite Ca <sub>5</sub> (PO <sub>4</sub> ) <sub>3</sub> OH	0
Vivianite Fe <sub>3</sub> (PO <sub>4</sub> ) <sub>2</sub> ·8H <sub>2</sub> O	0

It should be noted that the measured 66mg/L Cl is larger than the 13mg/L Cl computed using charge balance by Phreeqc. This charge balance discrepancy indicates either an error in the measurement of the dissolved constituents or that a significant analyte was not measured.

### 6.5.3 Discussion

From Table 13, as was also suggested by Strumm and Morgan (1981), we expect to see phosphate precipitate as hydroxyapatite, vivianite and MnHPO<sub>4</sub>. Sulfide metals such as chalcopyrite, pyrite, chalcocite, anilite, djurleite, blaubleill, blaubeil, covellite, greigite, millerite, sphalerite, mackinawite and FeS (ppt) are expected to precipitate out of the wastewater solution flowing through the wetland. In addition to this, nitrogen gas will be produced in the system.

The expected alkalinity from the phreeqc simulation for the wastewater flowing through the wetland is 4.41meq/L. This value is the same order of magnitude as the

alkalinity values observed in ponds, marshes and sewage leachate plumes in studies by Espinar & Serrano (2009) and by Lorah (2009). This could be explained by the fact that testing was performed in November, a month during which vegetation is dying and organics are collecting on the ground. In the case of the wetland around the C.K. Choi building, most of the wetland is covered with reeds during the summer months and starting around October, these plants begin to die and decompose on the gravel of the wetland system.

## **7. Discussion**

### **7.1 pH**

As is expected, the greywater is acidic because of the soap and the compost tea slightly basic to begin with. Standard freshwater has a pH of approximately 5.5 to 6 (Laurenzi 2010). The water flowing through the system should resemble that of standard freshwater since it is being cleaned by the wetland, so the pH of the wastewater was slightly acidic in March 2009, but was close to that of standard freshwater in November 2008. As the compost tea and greywater are mixed and begin to flow through the wetland system, the pH decreases from 7.71 in the compost tea to 6.04 at the furthest point from the building. This is as expected and is due to the oxidation of DOC increasing the concentration of  $H^+$  in the system. The drop in pH is also due to nitrification, consuming  $NH_4^+(aq)$  to produce  $H^+$ . The pH observed during sample collection (pH 6.04) is also close to the one output by the Phreeqc model (pH 6.054), which means that pH sampling was accurate.

## 7.2 Ammonia

Ammonia concentrations go from 692.9mg/L in the compost tea and 7.8mg/L in the greywater to 2.6mg/L at the sample tube closest to the building outlet to 5.4mg/L at the sample tube furthest from the building. This decrease is due to nitrification, converting  $\text{NH}_4^+(\text{aq})$  to nitrates.

## 7.3 Nitrate/Nitrite

$\text{NO}_x$  concentrations go from 307.7mg/L in the compost tea and 0.12mg/L in the greywater to 3.45mg/L at the sample tube closest to the building outlet to 3.30mg/L at the sample tube furthest from the building. This decrease is due to both dilution and denitrification. Denitrification uses  $\text{NO}_3^-$  and converts it to  $\text{N}_2$  gas. The nitrogen gas can then escape upwards through the soil and be released into the atmosphere. Formation of nitrogen gas is also also agrees with the Phreeqc analysis performed.

## 7.4 Mn(IV)-Fe(III) Reduction, Sulphate Reduction and Phosphorus Removal

Looking at the ICP results, we see a decrease in Mn, Fe and S concentrations. This is due to the oxidation of DOC and the reduction of metals and S listed in Table 3 and due to precipitation of Mn, Fe and S solids.

Manganese (IV) reduction uses some of the  $\text{H}^+$  produced from the denitrification process and converts the solid manganese dioxide, from the ground, into soluble Mn(II). Iron (III) reduction uses the solid phase iron hydroxide and  $\text{H}^+$  to produce aqueous Fe (II). Finally, sulfate reduction uses sulfate and converts it to hydrogen sulfide. This then facilitates the precipitation of metal-sulfides such as iron sulfide and also induces the

formation of sulfur gases that migrate up through the soil and diffuse in the atmosphere. Phreeqc also shows that many other sulfide metals will precipitate with metals such as copper, nickel and zinc (see Table 13 on page 32).

Soluble Mn and Fe, in addition to Ca, are easily adsorbed by phosphorus (Strumm and Morgan 1981). Phosphorus concentrations in the compost tea are high. As the liquid flows through the system, phosphorus is removed through bacterial removal, plant uptake, adsorption by the gravel and sand, and by precipitation.  $HPO_4^{2-}$  and  $H_2PO_4^-$  are the dominant forms of phosphate present at the pH conditions observed. Because of this, minerals such as hydroxyapatite,  $MnHPO_4$ , vivianite and strengite precipitate out of the solution.

## 8. Conclusion

Based upon the sampled analyzed, the wetlands processing the compost tea and greywater from the C.K. Choi building seem to be performing well. The concentrations of trace metals and minerals observed from the lab analyses agree well with the literature on wetland performance. It is expected that some trace metal concentrations will be lower than seen in other environments since the C.K. Choi building does not have many occupants, so wastewater concentrations are low to begin with. When the data from the compost tea was input in Phreeqc and simulated to run through an environment similar to that of the wetland, precipitate outputs also agreed with previous studies. Alkalinity, pH and metal concentrations are at levels that are normal and not harmful to the environment.

In further experiments, I would analyse the soil to observe what precipitates are present, so as to compare with the Phreeqc model. In this way, we could see whether some solids are present that are not available through the Phreeqc database and whether the precipitates identified with by Phreeqc are correct.

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## Appendix A: Lachat QuickChem FIA+ Analysis Methods

**Instrument:** Lachat QuickChem FIA+ (8000 series)

**Methods:** Chloride, nitrate/nitrite, low ammonia, low orthophosphate

**Applications:** Drinking, ground and surface waters, and domestic and industrial wastes

### QuickChem Methods Overview

Analyte	QuickChem Method #	Range (mg/L)	Detection Limits* (mg/L)
Ammonia (N as $\text{NH}_3^+$ )	10-107-06-2-A	0.1 – 5.00	0.005
Chloride (Cl <sup>-</sup> )	10-117-07-1-A	6 – 300	0.5
Nitrate / Nitrite (N as $\text{NO}_3^-$ / $\text{NO}_2^-$ )	12-107-04-1-B <sup>†</sup>	0.02 – 20.0	0.02
Orthophosphate (P as $\text{PO}_4^{3-}$ )	10-115-01-1-A	0.01 – 2.00	0.01

\* blanks should always be run with a sample set to determine any potential error or contamination from sample preparation (including filtration steps).

<sup>†</sup> Method for 2M KCl soil extracts, but used with a straight water matrix/carrier.

### Quality Control:

- Standard curves are re-run each day.
- During the run, a check standard is run every 10-15 samples to check for drift or other problems.

### Method descriptions:

(taken directly from QuickChem Methods)

Ammonia: When ammonia is heated with salicylate and hypochlorite in an alkaline phosphate buffer, an emerald green colour is produced which is proportional to the ammonia concentration. The colour is intensified by the addition of sodium nitroprusside.

Chloride: Chloride reacts with mercuric thiocyanate to form a strong, covalent complex which displaces thiocyanate. The free thiocyanate reacts with aqueous iron(III) to produce ferric thiocyanate (red colour), which absorbs strongly at 480 nm.

Nitrate: Nitrate is quantitatively reduced to nitrite by passage of the sample through a copperized cadmium column. The nitrite (reduced nitrate + original nitrite) is then determined by diazotizing with sulfanilamide followed by coupling with N-(1-

naphthyl)ethylenediamine dihydrochloride. The resulting water soluble dye has a magenta colour which is read at 520 nm.

Orthophosphate: The orthophosphate ion ( $\text{PO}_4^{3-}$ ) reacts with ammonium molybdate and antimony potassium tartrate under acidic conditions to form a complex. This complex is reduced with ascorbic acid to form a blue complex which absorbs light at 880 nm. The absorbance is proportional to the concentration of orthophosphate in the sample.

### **Potential interferences**

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Ammonia	<ol style="list-style-type: none"><li>1. In alkaline solution, Ca and Mg form a precipitate that scatters light (EDTA in buffer to prevent this).</li><li>2. Non-volatile amines such as cysteine, ethanolamine, and ethylenediamine cause decreased sensitivity.</li><li>3. Lauryl sulfate and some detergents can cause low recoveries.</li></ol>
Chloride	<ol style="list-style-type: none"><li>1. Substances that reduce iron(III) to iron(II) and mercury(III) to mercury(II) (e.g. sulfite, thiosulfate).</li><li>2. Other halides that form a strong complex with mercuric ion (e.g. <math>\text{Br}^-</math>, <math>\text{I}^-</math>).</li></ol>
Nitrate/Nitrite	<ol style="list-style-type: none"><li>1. Build up of suspended matter in column (pre-filter samples)</li><li>2. High concentrations of Fe, Cu, or other metals (EDTA in buffer to reduce this interference).</li><li>3. Large concentrations of oil and grease (must pre-extract sample with an organic solvent).</li></ol>
Orthophosphate	<ol style="list-style-type: none"><li>1. Silica forms a complex that also absorbs at 880 nm (generally an insignificant interference).</li><li>2. Concentrations of ferric iron (<math>\text{Fe}^{3+}</math>) &gt; 50 mg/L cause negative error due to precipitation of orthophosphate.</li><li>3. Sample turbidity.</li><li>4. Glassware contamination.</li></ol>

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V6T 1Z4*

Summary information compiled by T Naugler. January 13, 2009.

## Appendix B: ICP Data

Sampling Date	Location	Tube	Sample Labels	Mo 204.598	Cu 327.395	Cu 324.754	Mo 202.032	Zn 213.857	Zn 202.548	Zn 202.548	Cu 324.754
Nov-08	furthest from building	1 : 1	1a	0.015502	0.172134	0.219616	0.004884	1.2245	1.28063	1.28063	0.219616
Nov-08	closest to building	1 : 2	2a	0.02195	0.047343	0.096855	0.009299	0.381696	0.445887	0.445887	0.096855
Nov-08	compost tea	1 : 3	3a	0.511685	0.463857	0.72447	0.532739	0.741511	1.06938	1.06938	0.72447
Mar-09	furthest from building	1 : 4	1b	0.021174	0.019693	0.069954	0.009077	0.218021	0.277426	0.277426	0.069954
Mar-09	closest to building	1 : 5	2b	0.015817	0.067127	0.11485	0.009137	0.228709	0.286614	0.286614	0.11485

Sampling Date	Location	Tube	Sample Labels	Cr 267.716	As 193.696	As 188.980	Cr 276.653	Cr 205.560	Ni 230.299
Nov-08	furthest from building	1 : 1	1a	-0.031774	-0.005275	-0.064523	-0.012689	-0.017747	0.453686
Nov-08	closest to building	1 : 2	2a	-0.032141	0.008806	-0.074675	-0.013508	-0.019497	0.160351
Nov-08	compost tea	1 : 3	3a	-0.121301	0.17158	-0.032018	-0.047006	-0.064639	0.065269
Mar-09	furthest from building	1 : 4	1b	-0.032544	-0.002639	-0.074707	-0.013028	-0.017643	0.124578
Mar-09	closest to building	1 : 5	2b	-0.031231	0.006542	-0.062359	-0.012020	-0.018946	0.114064

Sampling Date	Location	Tube	Sample Labels	Ni 231.604	Ca 317.933	Ca 396.847	Ca 422.673	Fe 234.350	Fe 238.204	Fe 259.940	K 766.491
Nov-08	furthest from building	1 : 1	1a	0.43298	7.592	7.815	6.576	0.166	0.153	0.156	33.81
Nov-08	closest to building	1 : 2	2a	0.148449	6.026	6.225	5.115	0.325	0.318	0.319	27.9
Nov-08	compost tea	1 : 3	3a	-0.034293	156.3	145.2	145.9	9.961	10.16	10.11	6067 x
Mar-09	furthest from building	1 : 4	1b	0.114231	23.04	22.22	21.95	1.025	1.03	1.034	50.56
Mar-09	closest to building	1 : 5	2b	0.111669	16.42	16.12	15.11	0.211	0.201	0.206	42.67

Sampling Date	Location	Tube	Sample Labels	Mg 279.553	Mg 280.270	Mn 257.610	Mn 293.931	Na 588.995	Na 589.592	Si 212.412	Si 250.690
Nov-08	furthest from building	1 : 1	1a	-2.523	-0.161	0.452	0.452	38.57	36.17	-7.615	-7.935
Nov-08	closest to building	1 : 2	2a	-2.866	-0.438	0.424	0.424	38.85	36.42	-8.271	-8.611
Nov-08	compost tea	1 : 3	3a	-1.605	7.965	2.014	2.013	5910 x	5369 x	-29.81	-30.62
Mar-09	furthest from building	1 : 4	1b	2.202	3.588	0.468	0.467	94.58	91.87	-8.451	-8.782
Mar-09	closest to building	1 : 5	2b	0.001	1.858	0.441	0.439	81.74	79.77	-8.915	-9.267

Sampling Date	Location	Tube	Sample Labels	Se 203.985	Se 185.457	S 181.972	S 182.562	P 178.222	P 213.618	P 214.914
Nov-08	furthest from building	1 : 1	1a	0.033511	2.04771	3.54607	4.1466	5.707	5.331	5.353
Nov-08	closest to building	1 : 2	2a	0.044579	-3.08811	5.92219	6.75888	4.968	5.049	5.059
Nov-08	compost tea	1 : 3	3a	0.363731	9.93926	1133.11	1194.17	762.7	762.7	758.3
Mar-09	furthest from building	1 : 4	1b	0.057906	-1.40246	4.94004	5.7107	5.771	5.719	5.779
Mar-09	closest to building	1 : 5	2b	0.026885	1.34879	5.36984	5.49449	4.008	4.165	4.217

## Appendix C: Phreeqc Simulation Data

### Input File:

```
SELECTED_OUTPUT
-file thesis_trial1.xls
-water
-charge balance
-pH
-pe
-alkalinity
-percent_error
-totals      Cl S S(-2) S(6) N N(5) N(-3) N(3) N
             Ca Mg Na K
             Al Cu Fe Mn P Zn
-saturation_indices
  hydroxyapatite
  strengite
  vivianite
  hematite
  magnetite
  cupricFerrite
  Fe(OH)3(a)
  goethite
  maghemite
  MnHPO4

-equilibrium_phases
  strengite
  vivianite

PHASES
  Fix_H+
  H+ = H+
  log_k  0.0
```

```

# Water Type
SOLUTION 1
pH 7.71
Temp 25
pe 4
redox pe
units mg/L
density 1
Cl 3017 charge
S(6) 1133 as SO4
N(-3) 693 as N #NH4
N(5) 308 as N #NO3-
Ca 156
K 6067
Na 5910
Cu 0.4638
Fe 9.961
Mn 2.014
Ni 0.0653
P 762.7 as P
Zn 0.7415
-water 1 #kg
END

USE Solution 1
EQUILIBRIUM_PHASES 1
CO2(g) -3.5 10
siderite 0 0
hydroxyapatite 0 0
strengite 0 0
vivianite 0 0
ZnS(a) 0 0 0
Ni(OH)2 0 0
Calcite 0 0
SAVE EQUILIBRIUM_PHASES 2
SAVE SOLUTION 2
END

```

**Output File:**

Input file: E:\thesis\data\phreeqc trials\trial 2\Phrqcl\_t1.pqi  
Output file: E:\thesis\data\phreeqc trials\trial 2\Phrqcl\_t1.pqo  
Database file: C:\Program Files\USGS\Phreeqc Interactive 2.15.0\wateq4f.dat

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

SOLUTION\_MASTER\_SPECIES  
SOLUTION\_SPECIES  
PHASES  
EXCHANGE\_MASTER\_SPECIES  
EXCHANGE\_SPECIES  
SURFACE\_MASTER\_SPECIES  
SURFACE\_SPECIES  
RATES  
END

-----  
Reading input data for simulation 1.  
-----

DATABASE C:\Program Files\USGS\Phreeqc Interactive 2.15.0\wateq4f.dat  
SELECTED\_OUTPUT  
file thesis\_trial1.xls  
water  
charge\_balance balance  
ph  
pe  
alkalinity  
percent\_error  
totals Cl S S(-2) S(6) N N(5) N(-3) N(3) N  
Ca Mg Na K  
Al Cu Fe Mn P Zn  
saturation\_indices  
hydroxyapatite



```

strengite
vivianite
hematite
magnetite
cupricFerrite
Fe(OH)3(a)
goethite
maghemite
MnHPO4
equilibrium_phases
  strengite
  vivianite
PHASES
  Fix_H+
  H+ = H+
  log_k 0.0
SOLUTION 1
pH 7.71
Temp 25
pe 4
redox pe
units mg/L
density 1
Cl 3017 charge
S(6) 1133 as SO4
N(-3) 693 as N #NH4
N(5) 308 as N #NO3-
Ca 156
K 6067
Na 5910
Cu 0.4638
Fe 9.961
Mn 2.014
Ni 0.0653
P 762.7 as P
Zn 0.7415
water 1 #kg
END

```

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

Initial solution 1.

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

Elements	Molality	Moles	
Ca	3.964e-003	3.964e-003	
Cl	3.828e-001	3.828e-001	Charge balance
Cu	7.433e-006	7.433e-006	
Fe	1.816e-004	1.816e-004	
K	1.580e-001	1.580e-001	
Mn	3.733e-005	3.733e-005	
N(-3)	5.039e-002	5.039e-002	
N(5)	2.239e-002	2.239e-002	
Na	2.618e-001	2.618e-001	
Ni	1.133e-006	1.133e-006	
P	2.508e-002	2.508e-002	
S(6)	1.201e-002	1.201e-002	
Zn	1.155e-005	1.155e-005	

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

pH = 7.710  
pe = 4.000  
Activity of water = 0.985  
Ionic strength = 4.926e-001  
Mass of water (kg) = 1.000e+000  
Total alkalinity (eq/kg) = 2.417e-002  
Total carbon (mol/kg) = 0.000e+000  
Total CO2 (mol/kg) = 0.000e+000  
Temperature (deg C) = 25.000  
Electrical balance (eq) = -1.818e-015  
Percent error,  $100 * (\text{Cat} - |\text{An}|) / (\text{Cat} + |\text{An}|)$  = -0.00  
Iterations = 16

Total H = 1.112404e+002  
 Total O = 5.572208e+001

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

Redox couple	pe	Eh (volts)
N(-3)/N(5)	5.2077	0.3081

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	6.894e-007	5.055e-007	-6.162	-6.296	-0.135
H+	2.549e-008	1.950e-008	-7.594	-7.710	-0.116
H2O	5.551e+001	9.846e-001	1.744	-0.007	0.000
Ca	3.964e-003				
Ca+2	2.144e-003	5.599e-004	-2.669	-3.252	-0.583
CaHPO4	1.379e-003	1.545e-003	-2.860	-2.811	0.049
CaPO4-	2.557e-004	1.875e-004	-3.592	-3.727	-0.135
CaSO4	1.542e-004	1.728e-004	-3.812	-3.763	0.049
CaH2PO4+	3.088e-005	2.264e-005	-4.510	-4.645	-0.135
CaOH+	6.399e-009	4.692e-009	-8.194	-8.329	-0.135
CaHSO4+	2.692e-011	1.974e-011	-10.570	-10.705	-0.135
Cl	3.828e-001				
Cl-	3.828e-001	2.469e-001	-0.417	-0.608	-0.190
MnCl+	9.873e-006	7.239e-006	-5.006	-5.140	-0.135
CuCl2-	3.660e-006	2.683e-006	-5.437	-5.571	-0.135
CuCl3-2	3.633e-006	1.050e-006	-5.440	-5.979	-0.539
ZnCl+	1.932e-006	1.417e-006	-5.714	-5.849	-0.135
FeCl+	1.348e-006	9.884e-007	-5.870	-6.005	-0.135
ZnOHCl	7.858e-007	8.802e-007	-6.105	-6.055	0.049
MnCl2	6.964e-007	7.800e-007	-6.157	-6.108	0.049
ZnCl2	3.270e-007	3.663e-007	-6.485	-6.436	0.049
NiCl+	1.885e-007	1.382e-007	-6.725	-6.859	-0.135
ZnCl3-	1.384e-007	1.015e-007	-6.859	-6.994	-0.135
NiCl2	1.106e-007	1.239e-007	-6.956	-6.907	0.049

MnCl3-	7.233e-008	5.304e-008	-7.141	-7.275	-0.135
ZnCl4-2	4.343e-008	1.255e-008	-7.362	-7.901	-0.539
CuCl+	2.404e-009	1.763e-009	-8.619	-8.754	-0.135
CuCl2	2.086e-010	2.337e-010	-9.681	-9.631	0.049
CuCl3-	2.792e-013	2.047e-013	-12.554	-12.689	-0.135
FeCl+2	7.146e-014	2.065e-014	-13.146	-13.685	-0.539
FeCl2+	3.106e-014	2.277e-014	-13.508	-13.643	-0.135
CuCl4-2	8.763e-016	2.533e-016	-15.057	-15.596	-0.539
FeCl3	5.019e-016	5.622e-016	-15.299	-15.250	0.049
Cu(1)	7.292e-006				
CuCl2-	3.660e-006	2.683e-006	-5.437	-5.571	-0.135
CuCl3-2	3.633e-006	1.050e-006	-5.440	-5.979	-0.539
Cu+	1.899e-010	1.392e-010	-9.721	-9.856	-0.135
Cu(2)	1.406e-007				
Cu(OH)2	1.262e-007	1.413e-007	-6.899	-6.850	0.049
Cu+2	9.180e-009	2.653e-009	-8.037	-8.576	-0.539
CuCl+	2.404e-009	1.763e-009	-8.619	-8.754	-0.135
CuOH+	1.827e-009	1.340e-009	-8.738	-8.873	-0.135
CuSO4	7.480e-010	8.378e-010	-9.126	-9.077	0.049
CuCl2	2.086e-010	2.337e-010	-9.681	-9.631	0.049
Cu2(OH)2+2	2.717e-012	7.853e-013	-11.566	-12.105	-0.539
Cu(OH)3-	5.865e-013	4.300e-013	-12.232	-12.366	-0.135
CuCl3-	2.792e-013	2.047e-013	-12.554	-12.689	-0.135
CuCl4-2	8.763e-016	2.533e-016	-15.057	-15.596	-0.539
Cu(OH)4-2	1.499e-017	4.333e-018	-16.824	-17.363	-0.539
Fe(2)	6.718e-005				
FeHPO4	5.188e-005	5.812e-005	-4.285	-4.236	0.049
Fe+2	1.004e-005	2.901e-006	-4.998	-5.538	-0.539
FeH2PO4+	3.134e-006	2.298e-006	-5.504	-5.639	-0.135
FeCl+	1.348e-006	9.884e-007	-5.870	-6.005	-0.135
FeSO4	7.122e-007	7.978e-007	-6.147	-6.098	0.049
FeOH+	6.317e-008	4.632e-008	-7.199	-7.334	-0.135
Fe(OH)2	1.777e-011	1.991e-011	-10.750	-10.701	0.049
FeHSO4+	1.395e-013	1.022e-013	-12.856	-12.990	-0.135
Fe(OH)3-	5.094e-014	3.735e-014	-13.293	-13.428	-0.135
Fe(3)	1.145e-004				
Fe(OH)3	8.770e-005	9.823e-005	-4.057	-4.008	0.049
Fe(OH)2+	2.060e-005	1.510e-005	-4.686	-4.821	-0.135

Fe(OH)4-	6.170e-006	4.524e-006	-5.210	-5.345	-0.135
FeOH+2	3.125e-009	9.031e-010	-8.505	-9.044	-0.539
FeHPO4+	5.118e-012	3.752e-012	-11.291	-11.426	-0.135
FeH2PO4+2	4.078e-012	1.178e-012	-11.390	-11.929	-0.539
FeCl+2	7.146e-014	2.065e-014	-13.146	-13.685	-0.539
FeSO4+	6.407e-014	4.698e-014	-13.193	-13.328	-0.135
Fe+3	4.523e-014	2.770e-015	-13.345	-14.558	-1.213
FeCl2+	3.106e-014	2.277e-014	-13.508	-13.643	-0.135
Fe2(OH)2+4	3.147e-015	2.195e-017	-14.502	-16.659	-2.156
Fe(SO4)2-	2.168e-015	1.590e-015	-14.664	-14.799	-0.135
FeCl3	5.019e-016	5.622e-016	-15.299	-15.250	0.049
Fe3(OH)4+5	1.621e-016	6.926e-020	-15.790	-19.160	-3.369
FeHSO4+2	8.487e-021	2.453e-021	-20.071	-20.610	-0.539
H(0)	4.806e-027				
H2	2.403e-027	2.692e-027	-26.619	-26.570	0.049
K	1.580e-001				
K+	1.552e-001	1.001e-001	-0.809	-1.000	-0.190
KSO4-	1.483e-003	1.088e-003	-2.829	-2.963	-0.135
KHPO4-	1.340e-003	9.822e-004	-2.873	-3.008	-0.135
Mn(2)	3.733e-005				
Mn+2	2.491e-005	7.198e-006	-4.604	-5.143	-0.539
MnCl+	9.873e-006	7.239e-006	-5.006	-5.140	-0.135
MnSO4	1.767e-006	1.980e-006	-5.753	-5.703	0.049
MnCl2	6.964e-007	7.800e-007	-6.157	-6.108	0.049
MnCl3-	7.233e-008	5.304e-008	-7.141	-7.275	-0.135
MnOH+	1.274e-008	9.342e-009	-7.895	-8.030	-0.135
Mn(NO3)2	6.897e-009	7.725e-009	-8.161	-8.112	0.049
Mn(OH)3-	2.003e-017	1.469e-017	-16.698	-16.833	-0.135
Mn(3)	3.632e-026				
Mn+3	3.632e-026	2.224e-027	-25.440	-26.653	-1.213
Mn(6)	0.000e+000				
MnO4-2	0.000e+000	0.000e+000	-45.391	-45.930	-0.539
Mn(7)	0.000e+000				
MnO4-	0.000e+000	0.000e+000	-51.179	-51.314	-0.135
N(-3)	5.039e-002				
NH4+	4.849e-002	3.555e-002	-1.314	-1.449	-0.135
NH4SO4-	9.662e-004	7.084e-004	-3.015	-3.150	-0.135
NH3	9.277e-004	1.039e-003	-3.033	-2.983	0.049

N(5)	2.239e-002					
NO3-	2.239e-002	1.642e-002	-1.650	-1.785	-0.135	
Mn(NO3)2	6.897e-009	7.725e-009	-8.161	-8.112	0.049	
Na	2.618e-001					
Na+	2.574e-001	1.826e-001	-0.589	-0.738	-0.149	
NaHPO4-	2.444e-003	1.792e-003	-2.612	-2.747	-0.135	
NaSO4-	1.931e-003	1.416e-003	-2.714	-2.849	-0.135	
Ni	1.133e-006					
Ni+2	7.713e-007	2.229e-007	-6.113	-6.652	-0.539	
NiCl+	1.885e-007	1.382e-007	-6.725	-6.859	-0.135	
NiCl2	1.106e-007	1.239e-007	-6.956	-6.907	0.049	
NiSO4	6.002e-008	6.723e-008	-7.222	-7.172	0.049	
NiOH+	2.119e-009	1.554e-009	-8.674	-8.809	-0.135	
Ni(OH)2	5.075e-011	5.684e-011	-10.295	-10.245	0.049	
Ni(SO4)2-2	1.932e-011	5.584e-012	-10.714	-11.253	-0.539	
Ni(OH)3-	3.915e-014	2.870e-014	-13.407	-13.542	-0.135	
O(0)	9.960e-040					
O2	4.980e-040	5.578e-040	-39.303	-39.253	0.049	
P	2.508e-002					
HPO4-2	1.741e-002	5.033e-003	-1.759	-2.298	-0.539	
NaHPO4-	2.444e-003	1.792e-003	-2.612	-2.747	-0.135	
H2PO4-	2.156e-003	1.581e-003	-2.666	-2.801	-0.135	
CaHPO4	1.379e-003	1.545e-003	-2.860	-2.811	0.049	
KHPO4-	1.340e-003	9.822e-004	-2.873	-3.008	-0.135	
CaPO4-	2.557e-004	1.875e-004	-3.592	-3.727	-0.135	
FeHPO4	5.188e-005	5.812e-005	-4.285	-4.236	0.049	
CaH2PO4+	3.088e-005	2.264e-005	-4.510	-4.645	-0.135	
FeH2PO4+	3.134e-006	2.298e-006	-5.504	-5.639	-0.135	
PO4-3	1.900e-006	1.164e-007	-5.721	-6.934	-1.213	
FeHPO4+	5.118e-012	3.752e-012	-11.291	-11.426	-0.135	
FeH2PO4+2	4.078e-012	1.178e-012	-11.390	-11.929	-0.539	
S(6)	1.201e-002					
SO4-2	7.473e-003	1.547e-003	-2.127	-2.811	-0.684	
NaSO4-	1.931e-003	1.416e-003	-2.714	-2.849	-0.135	
KSO4-	1.483e-003	1.088e-003	-2.829	-2.963	-0.135	
NH4SO4-	9.662e-004	7.084e-004	-3.015	-3.150	-0.135	
CaSO4	1.542e-004	1.728e-004	-3.812	-3.763	0.049	
MnSO4	1.767e-006	1.980e-006	-5.753	-5.703	0.049	

FeSO4	7.122e-007	7.978e-007	-6.147	-6.098	0.049
ZnSO4	6.903e-007	7.732e-007	-6.161	-6.112	0.049
NiSO4	6.002e-008	6.723e-008	-7.222	-7.172	0.049
Zn(SO4)2-2	3.363e-008	9.720e-009	-7.473	-8.012	-0.539
HSO4-	3.999e-009	2.932e-009	-8.398	-8.533	-0.135
CuSO4	7.480e-010	8.378e-010	-9.126	-9.077	0.049
CaHSO4+	2.692e-011	1.974e-011	-10.570	-10.705	-0.135
Ni(SO4)2-2	1.932e-011	5.584e-012	-10.714	-11.253	-0.539
FeHSO4+	1.395e-013	1.022e-013	-12.856	-12.990	-0.135
FeSO4+	6.407e-014	4.698e-014	-13.193	-13.328	-0.135
Fe(SO4)2-	2.168e-015	1.590e-015	-14.664	-14.799	-0.135
FeHSO4+2	8.487e-021	2.453e-021	-20.071	-20.610	-0.539
Zn	1.155e-005				
Zn+2	7.379e-006	2.132e-006	-5.132	-5.671	-0.539
ZnCl+	1.932e-006	1.417e-006	-5.714	-5.849	-0.135
ZnOHCl	7.858e-007	8.802e-007	-6.105	-6.055	0.049
ZnSO4	6.903e-007	7.732e-007	-6.161	-6.112	0.049
ZnCl2	3.270e-007	3.663e-007	-6.485	-6.436	0.049
ZnOH+	1.610e-007	1.181e-007	-6.793	-6.928	-0.135
ZnCl3-	1.384e-007	1.015e-007	-6.859	-6.994	-0.135
Zn(OH)2	6.111e-008	6.845e-008	-7.214	-7.165	0.049
ZnCl4-2	4.343e-008	1.255e-008	-7.362	-7.901	-0.539
Zn(SO4)2-2	3.363e-008	9.720e-009	-7.473	-8.012	-0.539
Zn(OH)3-	1.491e-011	1.093e-011	-10.827	-10.961	-0.135
Zn(OH)4-2	3.027e-016	8.748e-017	-15.519	-16.058	-0.539

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

Phase	SI	log IAP	log KT	
Anhydrite	-1.70	-6.06	-4.36	CaSO4
Antlerite	-6.02	2.27	8.29	Cu3(OH)4SO4
Atacamite	-1.99	5.35	7.34	Cu2(OH)3Cl
Bianchite	-6.76	-8.52	-1.76	ZnSO4:6H2O
Birnessite	-9.92	33.68	43.60	MnO2
Bixbyite	-6.45	-7.07	-0.61	Mn2O3
Brochantite	-6.24	9.10	15.34	Cu4(OH)6SO4
Bunsenite	-3.69	8.76	12.45	NiO

Chalcanthite	-8.78	-11.42	-2.64	CuSO4:5H2O
Cu(OH)2	-1.81	6.83	8.64	Cu(OH)2
Cu2(OH)3NO3	-5.07	4.17	9.24	Cu2(OH)3NO3
Cu2SO4	-20.57	-22.52	-1.95	Cu2SO4
Cu3(PO4)2	-2.75	-39.60	-36.85	Cu3(PO4)2
Cu3(PO4)2:3H2O	-4.50	-39.62	-35.12	Cu3(PO4)2:3H2O
CuMetal	-5.10	-13.86	-8.76	Cu
CuOCuSO4	-16.08	-4.55	11.53	CuO:CuSO4
CupricFerrite	18.08	23.96	5.88	CuFe2O4
Cuprite	-2.75	-4.30	-1.55	Cu2O
CuprousFerrite	15.33	6.41	-8.92	CuFeO2
CuSO4	-14.40	-11.39	3.01	CuSO4
Fe(OH)2.7Cl.3	9.10	6.06	-3.04	Fe(OH)2.7Cl0.3
Fe(OH)3(a)	3.66	8.55	4.89	Fe(OH)3
Fe3(OH)8	6.75	26.97	20.22	Fe3(OH)8
Fix_H+	-7.71	-7.71	0.00	H+
Goethite	9.56	8.56	-1.00	FeOOH
Goslarite	-6.57	-8.53	-1.96	ZnSO4:7H2O
Gypsum	-1.50	-6.08	-4.58	CaSO4:2H2O
H2(g)	-23.42	-26.57	-3.15	H2
H2O(g)	-1.52	-0.01	1.51	H2O
Halite	-2.93	-1.35	1.58	NaCl
Hausmannite	-6.81	54.22	61.03	Mn3O4
Hematite	21.13	17.12	-4.01	Fe2O3
Hydroxyapatite	11.10	7.68	-3.42	Ca5(PO4)3OH
Jarosite(ss)	4.42	-5.41	-9.83	(K0.77Na0.03H0.2)Fe3(SO4)2(OH)6
Jarosite-K	5.14	-4.07	-9.21	KFe3(SO4)2(OH)6
Jarosite-Na	1.47	-3.81	-5.28	NaFe3(SO4)2(OH)6
JarositeH	-5.40	-10.79	-5.39	(H3O)Fe3(SO4)2(OH)6
Langite	-7.69	9.10	16.79	Cu4(OH)6SO4:H2O
Maghemite	10.74	17.12	6.39	Fe2O3
Magnetite	23.26	27.00	3.74	Fe3O4
Manganite	-3.37	21.97	25.34	MnOOH
Melanothallite	-13.52	-9.79	3.73	CuCl2
Melanterite	-6.19	-8.40	-2.21	FeSO4:7H2O
Mirabilite	-3.24	-4.35	-1.11	Na2SO4:10H2O
Mn2(SO4)3	-56.03	-61.74	-5.71	Mn2(SO4)3
Mn3(PO4)2	-5.47	-29.30	-23.83	Mn3(PO4)2



MnCl2:4H2O	-9.09	-6.38	2.71	MnCl2:4H2O
MnHPO4	5.51	-7.44	-12.95	MnHPO4
MnSO4	-10.62	-7.95	2.67	MnSO4
Morenosite	-7.15	-9.51	-2.36	NiSO4:7H2O
Nantokite	-3.70	-10.46	-6.76	CuCl
NH3(g)	-4.75	-2.98	1.77	NH3
Ni(OH)2	-2.05	8.75	10.80	Ni(OH)2
Ni3(PO4)2	-2.52	-33.82	-31.30	Ni3(PO4)2
Ni4(OH)6SO4	-15.20	16.80	32.00	Ni4(OH)6SO4
Nsutite	-8.88	33.68	42.56	MnO2
O2(g)	-36.36	-39.25	-2.89	O2
Portlandite	-10.65	12.15	22.80	Ca(OH)2
Pyrochroite	-4.94	10.26	15.20	Mn(OH)2
Pyrolusite	-7.70	33.68	41.38	MnO2
Retgersite	-7.46	-9.50	-2.04	NiSO4:6H2O
Strengite	4.89	-21.51	-26.40	FePO4:2H2O
Tenorite	-0.78	6.84	7.62	CuO
Thenardite	-4.11	-4.29	-0.18	Na2SO4
Vivianite	5.47	-30.53	-36.00	Fe3(PO4)2:8H2O
Zincite(c)	-1.40	9.74	11.14	ZnO
Zincosite	-11.49	-8.48	3.01	ZnSO4
Zn(NO3)2:6H2O	-12.72	-9.28	3.44	Zn(NO3)2:6H2O
Zn(OH)2-a	-2.71	9.74	12.45	Zn(OH)2
Zn(OH)2-b	-2.01	9.74	11.75	Zn(OH)2
Zn(OH)2-c	-2.46	9.74	12.20	Zn(OH)2
Zn(OH)2-e	-1.76	9.74	11.50	Zn(OH)2
Zn(OH)2-g	-1.97	9.74	11.71	Zn(OH)2
Zn2(OH)2SO4	-6.25	1.25	7.50	Zn2(OH)2SO4
Zn2(OH)3Cl	-4.04	11.16	15.20	Zn2(OH)3Cl
Zn3(PO4)2:4w	1.13	-30.91	-32.04	Zn3(PO4)2:4H2O
Zn3O(SO4)2	-26.24	-7.22	19.02	ZnO:2ZnSO4
Zn4(OH)6SO4	-7.68	20.72	28.40	Zn4(OH)6SO4
Zn5(OH)8Cl2	-6.44	32.06	38.50	Zn5(OH)8Cl2
ZnCl2	-13.92	-6.89	7.03	ZnCl2
ZnMetal	-39.43	-13.67	25.76	Zn
ZnO(a)	-1.57	9.74	11.31	ZnO
ZnSO4:H2O	-7.92	-8.49	-0.57	ZnSO4:H2O

-----  
End of simulation.  
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Reading input data for simulation 2.  
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```
USE Solution 1
EQUILIBRIUM_PHASES 1
CO2(g)      -3.5  10
siderite    0      0
hydroxyapatite 0      0
strengite   0      0
vivianite   0      0
ZnS(a)      0      0      0      0
Ni(OH)2     0      0
Calcite     0      0
SAVE EQUILIBRIUM_PHASES      2
SAVE SOLUTION      2
END
```

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

Reaction step 1.

Using solution 1.

Using pure phase assemblage 1.

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

Phase	SI	log IAP	log KT	Moles in assemblage		
				Initial	Final	Delta
Calcite	-4.78	-13.26	-8.48	0.000e+000	0	0.000e+000
CO2(g)	-3.50	-4.97	-1.47	1.000e+001	1.000e+001	-1.791e-005
Hydroxyapatite	-0.00	-3.42	-3.42	0.000e+000	6.008e-004	6.008e-004

Ni(OH)2	-5.36	5.44	10.80	0.000e+000	0	0.000e+000
Siderite	-4.44	-15.33	-10.89	0.000e+000	0	0.000e+000
Strengite	-4.15	-30.55	-26.40	0.000e+000	0	0.000e+000
Vivianite	0.00	-36.00	-36.00	0.000e+000	4.774e-005	4.774e-005
ZnS(a)	-0.66	-9.71	-9.05	0.000e+000	0	0.000e+000

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

Elements	Molality	Moles
C	1.789e-005	1.791e-005
Ca	9.588e-004	9.600e-004
Cl	3.823e-001	3.828e-001
Cu	7.424e-006	7.433e-006
Fe	3.838e-005	3.843e-005
K	1.578e-001	1.580e-001
Mn	3.729e-005	3.733e-005
N	7.269e-002	7.278e-002
Na	2.615e-001	2.618e-001
Ni	1.131e-006	1.133e-006
P	2.315e-002	2.318e-002
S	1.200e-002	1.201e-002
Zn	1.154e-005	1.155e-005

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

pH	=	6.054	Charge balance
pe	=	-2.435	Adjusted to redox equilibrium
Activity of water	=	0.985	
Ionic strength	=	4.388e-001	
Mass of water (kg)	=	1.001e+000	
Total alkalinity (eq/kg)	=	4.412e-003	
Total CO2 (mol/kg)	=	1.789e-005	
Temperature (deg C)	=	25.000	
Electrical balance (eq)	=	-1.536e-015	
Percent error, 100*(Cat- An )/(Cat+ An )	=	-0.00	
Iterations	=	25	
Total H	=	1.112390e+002	

Total O = 5.571354e+001

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

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	1.149e-006	8.834e-007	-5.940	-6.054	-0.114
OH-	1.527e-008	1.116e-008	-7.816	-7.952	-0.136
H2O	5.551e+001	9.851e-001	1.744	-0.007	0.000
C(-4)	2.775e-010				
CH4	2.775e-010	3.070e-010	-9.557	-9.513	0.044
C(4)	1.789e-005				
CO2	9.732e-006	1.077e-005	-5.012	-4.968	0.044
HCO3-	7.633e-006	5.340e-006	-5.117	-5.272	-0.155
NaHCO3	5.005e-007	5.537e-007	-6.301	-6.257	0.044
CaHCO3+	1.785e-008	1.306e-008	-7.748	-7.884	-0.136
MnHCO3+	4.618e-009	3.377e-009	-8.336	-8.471	-0.136
NaCO3-	1.331e-009	9.734e-010	-8.876	-9.012	-0.136
FeHCO3+	1.217e-009	8.897e-010	-8.915	-9.051	-0.136
CO3-2	1.184e-009	2.835e-010	-8.927	-9.547	-0.621
NiCO3	4.171e-010	4.614e-010	-9.380	-9.336	0.044
NiHCO3+	2.213e-010	1.618e-010	-9.655	-9.791	-0.136
MnCO3	1.444e-010	1.598e-010	-9.840	-9.796	0.044
CaCO3	8.230e-011	9.105e-011	-10.085	-10.041	0.044
FeCO3	1.024e-011	1.133e-011	-10.990	-10.946	0.044
ZnHCO3+	1.862e-015	1.362e-015	-14.730	-14.866	-0.136
Ni(CO3)2-2	7.948e-016	2.273e-016	-15.100	-15.643	-0.544
ZnCO3	1.036e-016	1.146e-016	-15.985	-15.941	0.044
Zn(CO3)2-2	2.428e-021	6.946e-022	-20.615	-21.158	-0.544
CuHCO3+	4.077e-022	2.981e-022	-21.390	-21.526	-0.136
CuCO3	1.533e-022	1.696e-022	-21.814	-21.771	0.044
Cu(CO3)2-2	2.116e-028	6.053e-029	-27.674	-28.218	-0.544
Ca	9.588e-004				
Ca+2	7.190e-004	1.917e-004	-3.143	-3.717	-0.574
CaH2PO4+	9.232e-005	6.752e-005	-4.035	-4.171	-0.136
CaHPO4	9.192e-005	1.017e-004	-4.037	-3.993	0.044
CaSO4	5.518e-005	6.105e-005	-4.258	-4.214	0.044

		3.724e-007	2.724e-007	-6.429	-6.565	-0.136
		1.785e-008	1.306e-008	-7.748	-7.884	-0.136
		4.320e-010	3.159e-010	-9.365	-9.500	-0.136
		8.230e-011	9.105e-011	-10.085	-10.041	0.044
		4.851e-011	3.548e-011	-10.314	-10.450	-0.136
Cl	3.823e-001					
		3.823e-001	2.497e-001	-0.418	-0.603	-0.185
		9.870e-006	7.218e-006	-5.006	-5.142	-0.136
		7.853e-007	5.743e-007	-6.105	-6.241	-0.136
		7.112e-007	7.868e-007	-6.148	-6.104	0.044
		1.883e-007	1.377e-007	-6.725	-6.861	-0.136
		1.129e-007	1.249e-007	-6.947	-6.904	0.044
		7.400e-008	5.412e-008	-7.131	-7.267	-0.136
		4.346e-010	1.243e-010	-9.362	-9.905	-0.544
		4.295e-010	3.141e-010	-9.367	-9.503	-0.136
		1.862e-012	1.362e-012	-11.730	-11.866	-0.136
		3.218e-013	3.561e-013	-12.492	-12.448	0.044
		1.364e-013	9.976e-014	-12.865	-13.001	-0.136
		4.365e-014	1.249e-014	-13.360	-13.904	-0.544
		1.689e-014	1.868e-014	-13.772	-13.729	0.044
		1.024e-019	7.487e-020	-18.990	-19.126	-0.136
		1.540e-020	4.404e-021	-19.813	-20.356	-0.544
		9.075e-021	1.004e-020	-20.042	-19.998	0.044
		6.717e-021	4.912e-021	-20.173	-20.309	-0.136
		1.109e-022	1.227e-022	-21.955	-21.911	0.044
		1.216e-023	8.896e-024	-22.915	-23.051	-0.136
		3.892e-026	1.113e-026	-25.410	-25.953	-0.544
Cu(1)	8.641e-010					
		4.346e-010	1.243e-010	-9.362	-9.905	-0.544
		4.295e-010	3.141e-010	-9.367	-9.503	-0.136
		2.178e-014	1.593e-014	-13.662	-13.798	-0.136
Cu(2)	7.423e-006					
		7.423e-006	5.428e-006	-5.129	-5.265	-0.136
		3.894e-019	1.114e-019	-18.410	-18.953	-0.544
		1.024e-019	7.487e-020	-18.990	-19.126	-0.136
		3.281e-020	3.630e-020	-19.484	-19.440	0.044
		9.075e-021	1.004e-020	-20.042	-19.998	0.044
		2.616e-021	2.894e-021	-20.582	-20.538	0.044

CuOH+	1.699e-021	1.242e-021	-20.770	-20.906	-0.136
CuHCO3+	4.077e-022	2.981e-022	-21.390	-21.526	-0.136
CuCO3	1.533e-022	1.696e-022	-21.814	-21.771	0.044
CuCl3-	1.216e-023	8.896e-024	-22.915	-23.051	-0.136
CuCl4-2	3.892e-026	1.113e-026	-25.410	-25.953	-0.544
Cu(OH)3-	2.659e-028	1.945e-028	-27.575	-27.711	-0.136
Cu(CO3)2-2	2.116e-028	6.053e-029	-27.674	-28.218	-0.544
Cu(OH)4-2	1.513e-034	4.328e-035	-33.820	-34.364	-0.544
Cu2(OH)2+2	2.361e-036	6.752e-037	-35.627	-36.171	-0.544
Fe(2)	3.838e-005				
FeH2PO4+	1.572e-005	1.149e-005	-4.804	-4.940	-0.136
Fe(HS)2	9.690e-006	1.072e-005	-5.014	-4.970	0.044
Fe+2	5.825e-006	1.666e-006	-5.235	-5.778	-0.544
FeHPO4	5.800e-006	6.417e-006	-5.237	-5.193	0.044
FeCl+	7.853e-007	5.743e-007	-6.105	-6.241	-0.136
FeSO4	4.274e-007	4.728e-007	-6.369	-6.325	0.044
Fe(HS)3-	1.356e-007	9.920e-008	-6.868	-7.004	-0.136
FeHCO3+	1.217e-009	8.897e-010	-8.915	-9.051	-0.136
FeOH+	8.034e-010	5.875e-010	-9.095	-9.231	-0.136
FeCO3	1.024e-011	1.133e-011	-10.990	-10.946	0.044
FeHSO4+	3.754e-012	2.746e-012	-11.425	-11.561	-0.136
Fe(OH)2	5.041e-015	5.577e-015	-14.298	-14.254	0.044
Fe(OH)3-	3.160e-019	2.311e-019	-18.500	-18.636	-0.136
Fe(3)	2.347e-015				
Fe(OH)2+	2.123e-015	1.553e-015	-14.673	-14.809	-0.136
Fe(OH)3	2.016e-016	2.231e-016	-15.695	-15.652	0.044
FeOH+2	1.470e-017	4.204e-018	-16.833	-17.376	-0.544
FeH2PO4+2	7.564e-018	2.163e-018	-17.121	-17.665	-0.544
Fe(OH)4-	3.102e-019	2.269e-019	-18.508	-18.644	-0.136
FeHPO4+	2.079e-019	1.521e-019	-18.682	-18.818	-0.136
FeCl+2	1.540e-020	4.404e-021	-19.813	-20.356	-0.544
FeSO4+	1.397e-020	1.022e-020	-19.855	-19.991	-0.136
Fe+3	9.759e-021	5.839e-022	-20.011	-21.234	-1.223
FeCl2+	6.717e-021	4.912e-021	-20.173	-20.309	-0.136
Fe(SO4)2-	4.879e-022	3.568e-022	-21.312	-21.448	-0.136
FeCl3	1.109e-022	1.227e-022	-21.955	-21.911	0.044
FeHSO4+2	8.451e-026	2.417e-026	-25.073	-25.617	-0.544
Fe2(OH)2+4	7.108e-032	4.758e-034	-31.148	-33.323	-2.174

Fe3(OH)4+5	0.000e+000	0.000e+000	-42.414	-45.812	-3.397
H(0)	7.415e-011				
H2	3.707e-011	4.101e-011	-10.431	-10.387	0.044
K	1.578e-001				
K+	1.560e-001	1.019e-001	-0.807	-0.992	-0.185
KSO4-	1.562e-003	1.143e-003	-2.806	-2.942	-0.136
KHPO4-	2.628e-004	1.922e-004	-3.580	-3.716	-0.136
Mn(2)	3.729e-005				
Mn+2	2.481e-005	7.095e-006	-4.605	-5.149	-0.544
MnCl+	9.870e-006	7.218e-006	-5.006	-5.142	-0.136
MnSO4	1.820e-006	2.014e-006	-5.740	-5.696	0.044
MnCl2	7.112e-007	7.868e-007	-6.148	-6.104	0.044
MnCl3-	7.400e-008	5.412e-008	-7.131	-7.267	-0.136
MnHCO3+	4.618e-009	3.377e-009	-8.336	-8.471	-0.136
MnOH+	2.781e-010	2.034e-010	-9.556	-9.692	-0.136
MnCO3	1.444e-010	1.598e-010	-9.840	-9.796	0.044
Mn(OH)3-	2.133e-022	1.560e-022	-21.671	-21.807	-0.136
Mn(NO3)2	0.000e+000	0.000e+000	-164.885	-164.842	0.044
Mn(3)	1.345e-032				
Mn+3	1.345e-032	8.047e-034	-31.871	-33.094	-1.223
Mn(6)	0.000e+000				
MnO4-2	0.000e+000	0.000e+000	-84.382	-84.925	-0.544
Mn(7)	0.000e+000				
MnO4-	0.000e+000	0.000e+000	-96.609	-96.745	-0.136
N(-3)	1.094e-002				
NH4+	1.072e-002	7.839e-003	-1.970	-2.106	-0.136
NH4SO4-	2.204e-004	1.612e-004	-3.657	-3.793	-0.136
NH3	4.571e-006	5.057e-006	-5.340	-5.296	0.044
N(0)	6.174e-002				
N2	3.087e-002	3.415e-002	-1.510	-1.467	0.044
N(3)	0.000e+000				
NO2-	0.000e+000	0.000e+000	-58.671	-58.807	-0.136
N(5)	0.000e+000				
NO3-	0.000e+000	0.000e+000	-80.010	-80.146	-0.136
Mn(NO3)2	0.000e+000	0.000e+000	-164.885	-164.842	0.044
Na	2.615e-001				
Na+	2.590e-001	1.844e-001	-0.587	-0.734	-0.148
NaSO4-	2.017e-003	1.475e-003	-2.695	-2.831	-0.136

NaHPO4-	4.757e-004	3.479e-004	-3.323	-3.459	-0.136
NaHCO3	5.005e-007	5.537e-007	-6.301	-6.257	0.044
NaCO3-	1.331e-009	9.734e-010	-8.876	-9.012	-0.136
Ni	1.131e-006				
Ni+2	7.676e-007	2.196e-007	-6.115	-6.658	-0.544
NiCl+	1.883e-007	1.377e-007	-6.725	-6.861	-0.136
NiCl2	1.129e-007	1.249e-007	-6.947	-6.904	0.044
NiSO4	6.176e-008	6.833e-008	-7.209	-7.165	0.044
NiCO3	4.171e-010	4.614e-010	-9.380	-9.336	0.044
NiHCO3+	2.213e-010	1.618e-010	-9.655	-9.791	-0.136
NiOH+	4.622e-011	3.380e-011	-10.335	-10.471	-0.136
Ni(SO4)2-2	2.048e-011	5.857e-012	-10.689	-11.232	-0.544
Ni(OH)2	2.468e-014	2.731e-014	-13.608	-13.564	0.044
Ni(CO3)2-2	7.948e-016	2.273e-016	-15.100	-15.643	-0.544
Ni(OH)3-	4.164e-019	3.045e-019	-18.380	-18.516	-0.136
O(0)	0.000e+000				
O2	0.000e+000	0.000e+000	-71.663	-71.619	0.044
P	2.315e-002				
H2PO4-	1.882e-002	1.377e-002	-1.725	-1.861	-0.136
HPO4-2	3.382e-003	9.675e-004	-2.471	-3.014	-0.544
NaHPO4-	4.757e-004	3.479e-004	-3.323	-3.459	-0.136
KHPO4-	2.628e-004	1.922e-004	-3.580	-3.716	-0.136
CaH2PO4+	9.232e-005	6.752e-005	-4.035	-4.171	-0.136
CaHPO4	9.192e-005	1.017e-004	-4.037	-3.993	0.044
FeH2PO4+	1.572e-005	1.149e-005	-4.804	-4.940	-0.136
FeHPO4	5.800e-006	6.417e-006	-5.237	-5.193	0.044
CaPO4-	3.724e-007	2.724e-007	-6.429	-6.565	-0.136
PO4-3	8.252e-009	4.938e-010	-8.083	-9.306	-1.223
FeH2PO4+2	7.564e-018	2.163e-018	-17.121	-17.665	-0.544
FeHPO4+	2.079e-019	1.521e-019	-18.682	-18.818	-0.136
S(-2)	7.752e-004				
H2S	5.932e-004	6.563e-004	-3.227	-3.183	0.044
HS-	1.162e-004	8.497e-005	-3.935	-4.071	-0.136
Zn(HS)2	1.152e-005	1.274e-005	-4.939	-4.895	0.044
Fe(HS)2	9.690e-006	1.072e-005	-5.014	-4.970	0.044
Cu(HS)3-	7.423e-006	5.428e-006	-5.129	-5.265	-0.136
Fe(HS)3-	1.356e-007	9.920e-008	-6.868	-7.004	-0.136
S5-2	5.781e-008	2.444e-008	-7.238	-7.612	-0.374



S4-2	3.795e-008	1.426e-008	-7.421	-7.846	-0.425
S6-2	2.728e-008	1.265e-008	-7.564	-7.898	-0.334
Zn(HS)3-	2.140e-008	1.565e-008	-7.670	-7.806	-0.136
S-2	4.062e-011	1.162e-011	-10.391	-10.935	-0.544
S3-2	1.562e-011	5.025e-012	-10.806	-11.299	-0.493
S2-2	1.033e-012	2.852e-013	-11.986	-12.545	-0.559
S(6)	1.122e-002				
SO4-2	7.364e-003	1.596e-003	-2.133	-2.797	-0.664
NaSO4-	2.017e-003	1.475e-003	-2.695	-2.831	-0.136
KSO4-	1.562e-003	1.143e-003	-2.806	-2.942	-0.136
NH4SO4-	2.204e-004	1.612e-004	-3.657	-3.793	-0.136
CaSO4	5.518e-005	6.105e-005	-4.258	-4.214	0.044
MnSO4	1.820e-006	2.014e-006	-5.740	-5.696	0.044
FeSO4	4.274e-007	4.728e-007	-6.369	-6.325	0.044
HSO4-	1.874e-007	1.371e-007	-6.727	-6.863	-0.136
NiSO4	6.176e-008	6.833e-008	-7.209	-7.165	0.044
CaHSO4+	4.320e-010	3.159e-010	-9.365	-9.500	-0.136
Ni(SO4)2-2	2.048e-011	5.857e-012	-10.689	-11.232	-0.544
FeHSO4+	3.754e-012	2.746e-012	-11.425	-11.561	-0.136
ZnSO4	6.852e-013	7.580e-013	-12.164	-12.120	0.044
Zn(SO4)2-2	3.438e-014	9.834e-015	-13.464	-14.007	-0.544
CuSO4	3.281e-020	3.630e-020	-19.484	-19.440	0.044
FeSO4+	1.397e-020	1.022e-020	-19.855	-19.991	-0.136
Fe(SO4)2-	4.879e-022	3.568e-022	-21.312	-21.448	-0.136
FeHSO4+2	8.451e-026	2.417e-026	-25.073	-25.617	-0.544
Zn	1.154e-005				
Zn(HS)2	1.152e-005	1.274e-005	-4.939	-4.895	0.044
Zn(HS)3-	2.140e-008	1.565e-008	-7.670	-7.806	-0.136
Zn+2	7.083e-012	2.026e-012	-11.150	-11.693	-0.544
ZnCl+	1.862e-012	1.362e-012	-11.730	-11.866	-0.136
ZnSO4	6.852e-013	7.580e-013	-12.164	-12.120	0.044
ZnCl2	3.218e-013	3.561e-013	-12.492	-12.448	0.044
ZnCl3-	1.364e-013	9.976e-014	-12.865	-13.001	-0.136
ZnCl4-2	4.365e-014	1.249e-014	-13.360	-13.904	-0.544
Zn(SO4)2-2	3.438e-014	9.834e-015	-13.464	-14.007	-0.544
ZnOHCl	1.689e-014	1.868e-014	-13.772	-13.729	0.044
ZnOH+	3.387e-015	2.477e-015	-14.470	-14.606	-0.136
ZnHCO3+	1.862e-015	1.362e-015	-14.730	-14.866	-0.136

ZnCO3	1.036e-016	1.146e-016	-15.985	-15.941	0.044
Zn(OH)2	2.867e-017	3.172e-017	-16.543	-16.499	0.044
Zn(CO3)2-2	2.428e-021	6.946e-022	-20.615	-21.158	-0.544
Zn(OH)3-	1.530e-022	1.119e-022	-21.815	-21.951	-0.136
Zn(OH)4-2	6.912e-029	1.977e-029	-28.160	-28.704	-0.544

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

Phase	SI	log IAP	log KT	
Anhydrite	-2.15	-6.51	-4.36	CaSO4
Anilite	8.43	-23.45	-31.88	Cu0.25Cu1.5S
Antlerite	-43.76	-35.47	8.29	Cu3(OH)4SO4
Aragonite	-4.93	-13.26	-8.34	CaCO3
Atacamite	-27.71	-20.37	7.34	Cu2(OH)3Cl
Azurite	-46.95	-43.20	3.75	Cu3(OH)2(CO3)2
Bianchite	-12.76	-14.53	-1.76	ZnSO4:6H2O
Birnessite	-29.42	14.18	43.60	MnO2
Bixbyite	-29.27	-29.89	-0.61	Mn2O3
BlaubleiI	6.33	-17.83	-24.16	Cu0.9Cu0.2S
BlaubleiII	6.85	-20.43	-27.28	Cu0.6Cu0.8S
Brochantite	-57.67	-42.33	15.34	Cu4(OH)6SO4
Bunsenite	-7.01	5.44	12.45	NiO
Calcite	-4.78	-13.26	-8.48	CaCO3
CH4(g)	-6.65	-9.51	-2.86	CH4
Chalcanthite	-19.14	-21.78	-2.64	CuSO4:5H2O
Chalcocite	9.01	-25.61	-34.62	Cu2S
Chalcopyrite	14.50	-20.77	-35.27	CuFeS2
CO2(g)	-3.50	-4.97	-1.47	CO2
Covellite	5.30	-16.97	-22.27	CuS
Cu(OH)2	-15.50	-6.86	8.64	Cu(OH)2
Cu2(OH)3NO3	-109.15	-99.91	9.24	Cu2(OH)3NO3
Cu2SO4	-28.44	-30.39	-1.95	Cu2SO4
Cu3(PO4)2	-38.62	-75.47	-36.85	Cu3(PO4)2
Cu3(PO4)2:3H2O	-40.37	-75.49	-35.12	Cu3(PO4)2:3H2O
CuCO3	-18.87	-28.50	-9.63	CuCO3
CuMetal	-2.60	-11.36	-8.76	Cu
CuOCuSO4	-40.13	-28.60	11.53	CuO:CuSO4

CupricFerrite	-18.90	-13.02	5.88	CuFe2O4
Cuprite	-13.94	-15.49	-1.55	Cu2O
CuprousFerrite	-1.91	-10.83	-8.92	CuFeO2
CuSO4	-24.76	-21.75	3.01	CuSO4
Djurleite	8.88	-25.04	-33.92	Cu0.066Cu1.868S
Fe(OH)2.7Cl.3	-2.05	-5.09	-3.04	Fe(OH)2.7Cl0.3
Fe(OH)3(a)	-7.98	-3.09	4.89	Fe(OH)3
Fe3(OH)8	-20.09	0.13	20.22	Fe3(OH)8
FeS(ppt)	0.12	-3.80	-3.92	FeS
Fix_H+	-6.05	-6.05	0.00	H+
Goethite	-2.09	-3.09	-1.00	FeOOH
Goslarite	-12.58	-14.54	-1.96	ZnSO4:7H2O
Greigite	4.72	-40.31	-45.03	Fe3S4
Gypsum	-1.95	-6.53	-4.58	CaSO4:2H2O
H2(g)	-7.24	-10.39	-3.15	H2
H2O(g)	-1.52	-0.01	1.51	H2O
H2S(g)	-2.19	-3.18	-1.00	H2S
Halite	-2.92	-1.34	1.58	NaCl
Hausmannite	-32.94	28.09	61.03	Mn3O4
Hematite	-2.16	-6.16	-4.01	Fe2O3
Hydroxyapatite	-0.00	-3.42	-3.42	Ca5(PO4)3OH
Jarosite(ss)	-25.18	-35.01	-9.83	(K0.77Na0.03H0.2)Fe3(SO4)2(OH)6
Jarosite-K	-24.79	-34.00	-9.21	KFe3(SO4)2(OH)6
Jarosite-Na	-28.47	-33.75	-5.28	NaFe3(SO4)2(OH)6
JarositeH	-33.68	-39.07	-5.39	(H3O)Fe3(SO4)2(OH)6
Langite	-59.12	-42.33	16.79	Cu4(OH)6SO4:H2O
Mackinawite	0.85	-3.80	-4.65	FeS
Maghemite	-12.55	-6.16	6.39	Fe2O3
Magnetite	-3.58	0.16	3.74	Fe3O4
Malachite	-30.18	-25.03	5.15	Cu2(OH)2CO3
Manganite	-14.78	10.56	25.34	MnOOH
Melanothallite	-23.89	-20.16	3.73	CuCl2
Melanterite	-6.41	-8.62	-2.21	FeSO4:7H2O
Millerite	3.37	-4.68	-8.04	NiS
Mirabilite	-3.22	-4.33	-1.11	Na2SO4:10H2O
Mn2(SO4)3	-68.87	-74.58	-5.71	Mn2(SO4)3
Mn3(PO4)2	-10.23	-34.06	-23.83	Mn3(PO4)2
MnCl2:4H2O	-9.09	-6.38	2.71	MnCl2:4H2O

MnHPO4	4.78	-8.16	-12.95	MnHPO4
MnS(Green)	-6.97	-3.17	3.80	MnS
MnSO4	-10.61	-7.95	2.67	MnSO4
Morenosite	-7.14	-9.50	-2.36	NiSO4:7H2O
N2(g)	1.79	-1.47	-3.26	N2
Nahcolite	-5.46	-6.01	-0.55	NaHCO3
Nantokite	-7.64	-14.40	-6.76	CuCl
Natron	-9.77	-11.08	-1.31	Na2CO3:10H2O
NH3(g)	-7.07	-5.30	1.77	NH3
Ni(OH)2	-5.36	5.44	10.80	Ni(OH)2
Ni3(PO4)2	-7.29	-38.59	-31.30	Ni3(PO4)2
Ni4(OH)6SO4	-25.15	6.85	32.00	Ni4(OH)6SO4
NiCO3	-9.37	-16.21	-6.84	NiCO3
Nsutite	-28.38	14.18	42.56	MnO2
O2(g)	-68.73	-71.62	-2.89	O2
Portlandite	-14.42	8.38	22.80	Ca(OH)2
Pyrite	11.80	-6.68	-18.48	FeS2
Pyrochroite	-8.25	6.95	15.20	Mn(OH)2
Pyrolusite	-27.20	14.18	41.38	MnO2
Retgersite	-7.45	-9.49	-2.04	NiSO4:6H2O
Rhodochrosite	-3.57	-14.70	-11.13	MnCO3
Rhodochrosite(d)	-4.31	-14.70	-10.39	MnCO3
Siderite	-4.44	-15.33	-10.89	FeCO3
Siderite(d)(3)	-4.88	-15.33	-10.45	FeCO3
Smithsonite	-11.24	-21.24	-10.00	ZnCO3
Sphalerite	1.91	-9.71	-11.62	ZnS
Strengite	-4.15	-30.55	-26.40	FePO4:2H2O
Sulfur	-0.78	-15.81	-15.03	S
Tenorite	-14.47	-6.85	7.62	CuO
Thenardite	-4.09	-4.27	-0.18	Na2SO4
Thermonatrite	-11.15	-11.02	0.13	Na2CO3:H2O
Trona	-16.24	-17.04	-0.80	NaHCO3:Na2CO3:2H2O
Vivianite	0.00	-36.00	-36.00	Fe3(PO4)2:8H2O
Wurtzite	-0.03	-9.71	-9.68	ZnS
Zincite(c)	-10.73	0.41	11.14	ZnO
Zincosite	-17.50	-14.49	3.01	ZnSO4
Zn(NO3)2:6H2O	-175.46	-172.02	3.44	Zn(NO3)2:6H2O
Zn(OH)2-a	-12.05	0.40	12.45	Zn(OH)2

Zn(OH)2-b	-11.35	0.40	11.75	Zn(OH)2
Zn(OH)2-c	-11.80	0.40	12.20	Zn(OH)2
Zn(OH)2-e	-11.10	0.40	11.50	Zn(OH)2
Zn(OH)2-g	-11.31	0.40	11.71	Zn(OH)2
Zn2(OH)2SO4	-21.59	-14.09	7.50	Zn2(OH)2SO4
Zn2(OH)3Cl	-21.05	-5.85	15.20	Zn2(OH)3Cl
Zn3(PO4)2:4w	-21.68	-53.72	-32.04	Zn3(PO4)2:4H2O
Zn3O(SO4)2	-47.59	-28.57	19.02	ZnO:2ZnSO4
Zn4(OH)6SO4	-41.69	-13.29	28.40	Zn4(OH)6SO4
Zn5(OH)8Cl2	-49.79	-11.29	38.50	Zn5(OH)8Cl2
ZnCl2	-19.93	-12.90	7.03	ZnCl2
ZnCO3:H2O	-10.99	-21.25	-10.26	ZnCO3:H2O
ZnMetal	-32.58	-6.82	25.76	Zn
ZnO(a)	-10.90	0.41	11.31	ZnO
ZnS(a)	-0.66	-9.71	-9.05	ZnS
ZnSO4:H2O	-13.93	-14.50	-0.57	ZnSO4:H2O

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